THE DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS

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THE DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS

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LIST OF SYMBOLS AND ABBREVIATIONS

d_i^+, d_i^-	Deviation variables in cDSP
EMI	Error Margin Index
$HD-EMI$	Hyper-Dimensional Error Margin Index
Ns	Number of sample points
R	Correlation matrix
$\hat{y}$	Predicted estimates of the response
r^T	Correlation vector of length n_s
α	value of bandwidth; smoothing parameter
$\boldsymbol{X}$	Design matrix
$\boldsymbol{W}$	Diagonal matrix
$\boldsymbol{L}$	Hat matrix
$PMSE$	Prediction mean squared error
CV	Cross validation
$\hat{\mu}_{-i}$	Leave-x_i-out estimate of $\mu(x_i)$
GCV	Generalized cross validation
$\hat{\mu}$	Local estimate
ν	Fitted degrees of freedom
dx	Size of design freedom
f_0, y_0	Mean response model
f_i	Uncertainty bound functions
$Y_{\max}$, y_{max}	Upper boundary of response boundary
$Y_{\min}$, y_{min}	Lower boundary of response boundary
xl	Lower boundary of the design variable range

xu	Upper boundary of the design variable range
$f_{upper95\%}$, $f_{lower95\%}$	95% confidence interval
URL	Upper requirement limit
LRL	Lower requirement limit
w_i	Weight of design goal i
Z	Deviation function in cDSP
σ_{yy}	Initial loading
T_{ignit}	Weighted average of temperatures of local hot spots at a first reaction initiation
T	Temperature of a hot spot
A	Size of a hot spot
rh	radius of the air holes in waveguide
np	number of periods in coupler
cr	change rate of the air holes in coupler
$Twaveguide$	Transmission of waveguide
$Tsystem$	Transmission of system

SUMMARY

The design exploration method for adaptive design systems is developed to facilitate the pursuit of a balance between the efficiency and accuracy in systems engineering design. The proposed method is modified from an existing multiscale material robust design method, the Inductive Design Exploration Method (IDEM). The IDEM is effective in managing uncertainty propagation in the model chain. However, it is not an appropriate method in other systems engineering design outside of original design domain due to its high computational cost. In this thesis, the IDEM is augmented with more efficient solution search methods to improve its capability for efficiently exploring robust design solutions in systems engineering design.

The accuracy of the meta-model in engineering design is one uncertainty source. In current engineering design, response surface model is widely used. However, this method is shown as inaccurate in fitting nonlinear models. In this thesis, the local regression method is introduced as an alternative of meta-modeling technique to reduce the computational cost of simulation models. It is proposed as an appropriate method in systems design with nonlinear simulations models.

The proposed methods are tested and verified by application to a Multifunctional Energetic Materials design and a Photonic Crystal Coupler and Waveguide design. The methods are demonstrated through the better accuracy of the local regression model in comparison to the response surface model and the better efficiency of the design exploration method for adaptive design systems in comparison to the IDEM. The proposed methods are validated theoretically and empirically through application of the validation square.

CHAPTER 1
FOUNDATION OF SYSTEMS DESIGN

In this thesis, the design exploration method for adaptive design systems (DEM-ADS) is developed and implemented to facilitate the design of the simulation-based Multifunctional Energetic Structural Materials (MESMs) and the design of the Photonic Crystal Coupler and Waveguide (PCCW). The proposed method is applied to provide designers with a ranged set of design solutions which are robust to the different types of uncertainties existing in the system.

The core step in DEM-ADS is the inverse design exploration, which is modified from an existing robust design approach for multiscale material design, the Inductive Design Exploration Method (IDEM). The DEM-ADS is proposed to manage the uncertainty in complex systems and solve the design problems efficiently. It addressed a set of limitations associated with meta-modeling techniques and existing robust design methods, including the IDEM, which are discussed in detail in Chapter 2.

Development of the DEM-ADS is motivated by the need for efficient design approach for systems design, which is usually computationally intensive and contains different types of uncertainties. A robust design approach for systems design must facilitate balancing the efficiency of design exploration against the uncertainty due to model simplification. By employing the DEM-ADS including an inverse design procedure with efficient solution search methods and appropriate data-fitting method, the contributions are made to the domain of systems design, especially adaptive design systems. First, the DEM-ADS provides designers with the possibilities to solve more complex design problems with less computational cost than an existing robust design approach, the IDEM, when design information is sufficient, such as adaptive design systems. Second, the local regression provides designers with an alternative to fit highly nonlinear models in the design process.

The research described in this thesis is motivated by a set of challenges associated with systems design and a set of limitations associated with existing robust design approaches. Chapter 1 begins with a description of systems design motivation. In Section 1.2, the frame of reference for this thesis is established with a discussion of robust design approaches and the meta-modeling techniques. In Section 1.3, the research focus of this thesis is presented, including the primary and secondary research questions and hypotheses. Research contributions from this thesis are also discussed. Chapter 1 concludes with the introduction of the design method validation strategy used in this thesis in Section 1.4, and finally, in Section 1.5, a roadmap for the thesis is provided.

1.1 MOTIVATION FOR DEVELOPING THE ROBUST DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS

With the current trend of increasing product performance requirements, many design problems become more complex, including both the coupling between system components and couplings in different physical phenomena and time scales. Such complexities cause design challenges such as solution search efficiency and uncertainty management. It is necessary to develop a robust design approach to address these challenges. In Section 1.1, an overview of the complex system and the key challenges faced in complex system design are given.

1.1.1 The Definition of the System

There are a lot of different definitions of "system". According to Wikipedia, "*system is a set of interacting or interdependent entities, real or abstract, forming an integrated* *whole*". In Encyclopedia [1], system is defined as "*aggregation of things so combined to form an integral or complex whole*". In Electronic Terms of IEEE[2], system is defined as "*combination of components that act together to perform a function not possible with any of individuals parts*". These definitions share the same common characteristics, including the following:

- A system works as a whole entity and has specific functions;
- A system has different components, which interact with each other;
- A system has a clear structure.

In this thesis, system is defined as "**a combination of interacting entities with a clear structure and specific boundary which performs specific functions**". The boundary defines the scope of a system, which separates the inside entities and outside environment. In engineering design, environment is usually considered as an important factor influencing the performance of a system. Therefore, the system defined in this thesis is also open to effects from the environment different from the "closed system" that is isolated from its environment. The system design should take both inside and outside factors into consideration. One important outside factor is the uncertainty, which is discussed in details in Section 1.1.4.

One complexity of the system comes from the large number of multiple interactions between subsystems, components, or interactions happening on different scales in the same subsystem. It is not exaggerating to say that most of engineering design problems are system design problems. For instance, the design of an automobile involves design of the systems such as engine, transmission, cooling, body and their integration. Each of these components is actually another complex system. For instance, a transmission system consists of an arrangement of gears, brakes, a fluid drive and etc. Therefore, in order to analyze the complex system problem, both interactions between different subsystems and internal structure of each subsystem should be carefully studied. In this thesis, the interaction which happens between subsystems is called *single-level coupling*. For instance, in the automobile system, the interaction between engine and transmission is a single-level coupling. The interaction which happens between a subsystem and its own sub-subsystems is called *multi-level coupling*. This kind of coupling usually happens when design problems can be analyzed at various length and/ or time scales. The system shown in Figure 1. 1 is one complex system. The system has a boundary which separate internal components and outside environment. Each component in this system is a subsystem, which may contain other mini-systems, or called sub-subsystems. Subsystem 1, 2 and 3 have interaction between each other and Subsystem 3 outputs the whole system performance. The interactions in Subsystem 1, 2 and 3 are single-level couplings. In Subsystem 1, there is a mini-system structure. The output of SS1 and SS2 become an input for the Subsystem 1. The mini-system consisting of SS1 and SS2 is a micro-level and happens in different various length and/ or time interval from Subsystem 1. Such interaction is the multi-level coupling. This kind of coupling is common in material design.

The strengths of each of these couplings are different in different design problems. Some of the couplings are weak and may be ignored during modeling and design. Meanwhile, others are strong and must be considered [3]. In material design, the strength of multi-level couplings is very high. In this thesis, both single-level couplings and multi-level couplings are considered as important factors for decision making in systems design.

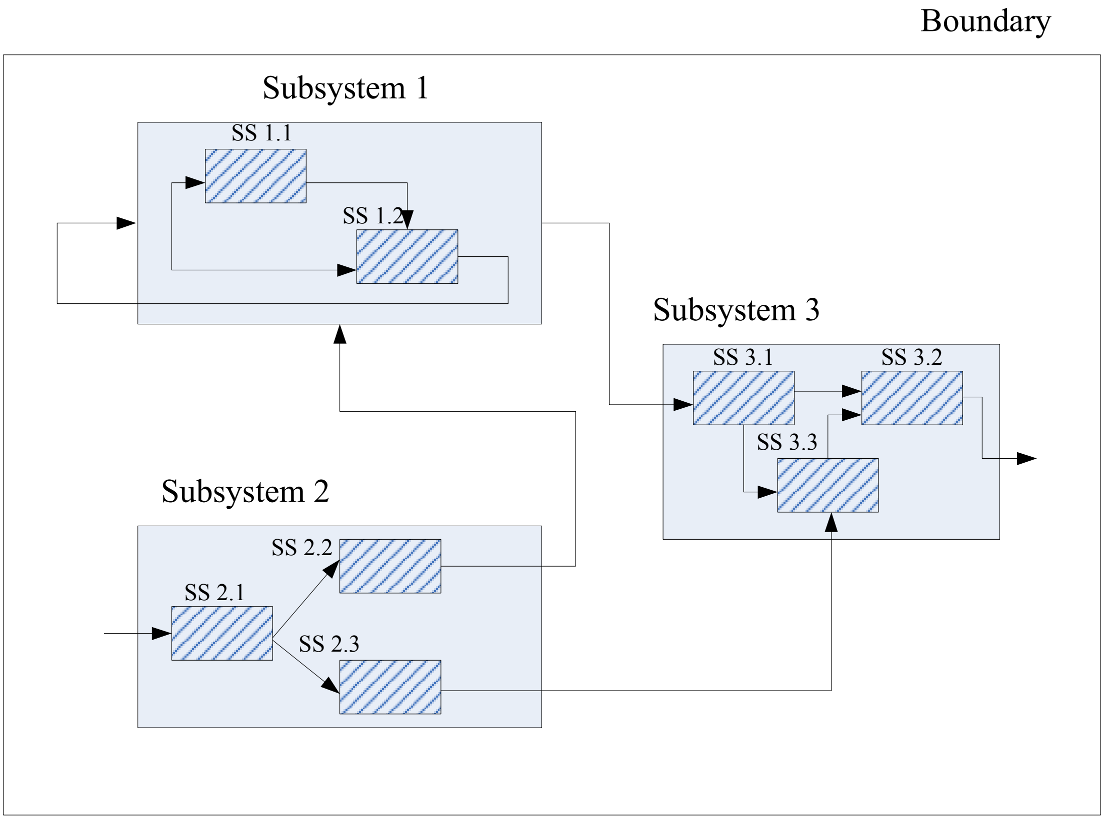


Figure 1. 1 - An example of complex systems

1.1.2. Example of System Design – Material Design

This section is leveraged from Hae-Jin Choi's Ph.D. dissertation [4] with modifications.

Material design is one of the most important challenges in the application of complex system design. For thousands of years, the technology developments have been closely linked to the availability of materials. The Information Age is actually built on the critical advance in semiconductors and other materials which make information technology revolution possible. However, the materials are not designed; instead, they are selected from a database of available options [5]. Currently, many complex new products systems requires increasing more sophisticated properties, such as high temperature and high pressure, which unfortunately may not always be available in current material selections.

The main difficulty with material selection is that the materials cannot be tailored to application-specific requirements. On the other hand, the development of new materials usually takes a relatively long time compared to the product development circle for new products. Material design techniques offer the potential for tailoring materials for challenging applications. Materials are no longer only selected from a database. The material structure and processing paths are tailored to achieve properties and performances for a particular application [6].

Materials design offers the potential for alleviating the limitation of current material technology. However, materials design is challenging. Materials are multi-scale and hierarchical systems with phenomena and materials design opportunities manifested on a hierarchy of length and time intervals from atomic scales to component length scales [6]. As shown in Figure 1. 2, the engine system is one subsystem in the complex airplane system design. The performance of the engine is determined by the material design in different length and time levels. For instance, the microstructures of the materials will influence the limitations of maximum heat tolerance of the engine which will become important design information for the engine system design. This interaction happens at different length and time levels, so that it is a typical multi-level coupling in complex systems design.

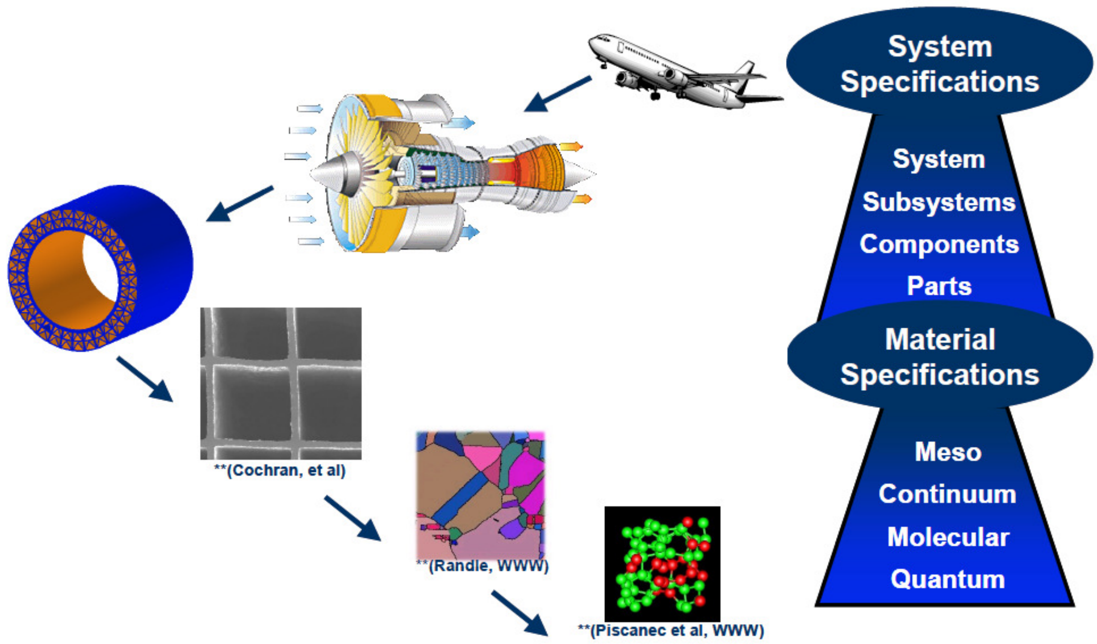


Figure 1. 2 - Material design as a complex system design [6]

Current material design processes are deductive in nature (bottom-up), in which the process path of a material can adjust the microstructure and the adjustment of the microstructure can change the properties and performance of the material. From engineering design perspective, it is advantageous for material design processes to consist of an inductive (top-down) approach in which designers specify the required material performance at the beginning of the design process [7]. The property, microstructure and processing will be determined by the material performance requirements. The material design process is shown in Figure 1. 3.

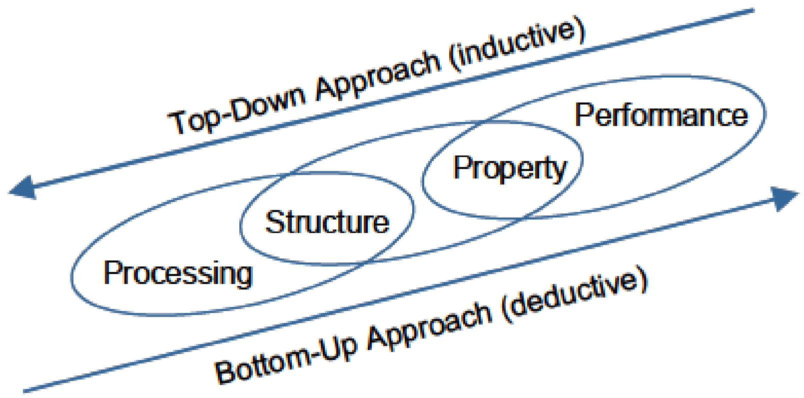


Figure 1. 3 - Materials design process [8]

Material design is very complex due to lack of sufficient information in the design problem. Material designers have to identify new knowledge while solving the design problems. The complexity of this kind of systems design comes from the uncertain subsystem functions and uncertain coupling relationships. However, not all of systems design problems have the same complexity. In the next section, different types of design problem are introduced. Each type of design problem involves different complexity so that designers should implement different solution search strategy to solve design problems.

1.1.3 Design Types

In terms of design novelty, design problems can be classified as original design, adaptive design, and variant design [9]. Different types of design determine different amounts of design information available for designers, which require the design techniques to be employed. In this section, different design types are introduced.

In the original design, original principles are determined for a desired system and then used to create a product. It can be realized either by selecting and combining known principles and technology or inventing completely new technology. Materials design is one example of original design. Instead of choosing different materials, material design techniques satisfy challenging design requirements by tailoring currently available materials. In this kind of original design, the mapping function of the input and output in a subsystem may be unknown. Therefore, designers may have to explore the whole design space to obtain the mapping relationship by expensive experiments. Moreover, the product of the original design may be uncertain. Due to lack of sufficient information about the new technology or too many constraints existing, designers are not sure if the desired objectives are reasonable. In this case, designers also have to check the whole design space to check the feasibilities.

In adaptive design, an existing design is adapted to different conditions or tasks. In this case, the solution principles are kept the same and no new principles are developed, but the product will be sufficiently different so that it can meet the changed tasks that have been specified. Most current design problems belong to the adaptive design and geometrical, analytical and production issues are the emphasis [9]. The mapping relationship of each subsystem is available, and design information is also sufficient for designers to correctly define the design objectives and identify all design constraints. Therefore, in adaptive design, it is not necessary to explore the whole design space. Instead, it is necessary for designers to identify the couplings in the system, so that the main task to the designers becomes to manage the complexity arising from the complex multiple interactions. In this thesis, adaptive design is the focus and sufficient information should be available to the designers.

In variant design, the sizes and arrangements of parts and system components are varied within the limits set by the previously designed product structure. It includes designs in which only the dimensions of individual parts are modified to meet a specific requirement. Product family design and modular product design are examples of variant design. Therefore, in this case, designers have more design information than the other design types.

In reality, it is difficult to clearly define the boundary between three types of design[9]. In this thesis, adaptive design is the emphasis, in which designers have sufficient information to clearly identify design objectives and design constraints. In addition, simulation models are available, and designers have knowledge about the models so that reasonable and achievable design objectives can be defined. Therefore, in adaptive design environment, it is not necessary to implement discrete exploration in the whole design space and efficient solution search methods can be employed to find design specifications.

1.1.4 Systems Design Challenges

In the adaptive design systems, designers have more design information or knowledge about subsystems and system function than the original design. The mapping relationship between inputs and outputs in each subsystem is known, so that the design objectives determined based on available design information are reasonable and achievable. However, there are still several of the key challenges in systems design to be addressed. In this section, the systems design challenges are studied. These challenges are addressed in the robust design approach and meta-modeling techniques for systems presented in Chapter 3.

The primary design challenge due to the complex nature of system design problems comes from two kinds of couplings, single-level couplings and multi-level couplings, which are necessary for designers to appropriately account for the couplings that affect the ultimate behavior of the complete system. The objective in designing is to utilize information generated by complex models in a goal-oriented manner to realize all requirements. Current methods in simulation-based system design do not encompass the full set of performance criteria to produce better designs considering variables from all levels – material microstructure through overall system [10]. Design of complex systems is characterized by the challenges of complex system modeling and additional challenges associated with design exploration at different subsystem levels and couplings. The challenges in complex system design are leveraged from Jitesh Panchal's PhD dissertation [3] and are presented as follow:

Increased number of design variables and couplings: (why efficient solution method is necessary) Couplings between complex system models induce complexity in the associated design processes, which is further increased if the design is multi-functional. Complex, multi-functional design processes involve different domain experts with distributed simulation models. All these factors further complicate the design processes. In order to reduce the complexity of design processes, it is important that only the couplings that are most important for decision making be considered in the design process. The efficient computational methods should also be considered in order to keep the computational cost at an affordable level.

Decision-making under uncertainty: (why local regression is necessary) Uncertainty in design of complex systems arises from three sources – a) inherent randomness in the system, b) lack of knowledge about the system, and c) the error introduced in the models due to simplification of simulation models and design process. Effective management of uncertainty involves making decisions robust to uncertainty in the simulation models and mitigating uncertainty through model refinement. Proper accounting for uncertainty is especially important in complex design because of the propagation of uncertainty across different models and scales. Design methods for robust decision making under uncertainty and propagated uncertainty are required.

Decision exploration techniques: (why the overall robust design approach for complex systems) Complex problems are generally characterized by an increase in number of parameters that can be modified to achieve design goals. This increases the efforts for design exploration using conventional techniques. This calls for the development of faster and more efficient design exploration techniques. These include design of computer experiments, approximation techniques, etc. Further, complex system design problems are characterized by long simulation runtime and large degrees of freedom. Using such models in the design exploration loops is computationally prohibitive. Hence, efficient design of experiments and meta-modeling techniques are required to create simplified mathematical relationships between the design variables and responses that can be used for design space exploration.

Based on the challenges in complex systems design, the requirements list for a robust design approach for complex systems is shown in the Table 1. 1.

Table 1. 1 - Requirements list for a robust design approach for complex systems

<table>
<tr><th colspan="3">Requirements list for complex systems design</th><th>Issued On:
2/18/2009</th></tr>
<tr><td colspan="4">Problem Statements:
Explore a design approach for complex systems that facilitates design decision-making and addresses the critical challenges identified in complex systems design.</td></tr>
<tr><th>#</th><th>Demand/Wish</th><th colspan="2">Requirements</th></tr>
<tr><td colspan="4">Complexity Management</td></tr>
<tr><td>1</td><td>D</td><td colspan="2">Only important design variables and couplings should be considered in the design process</td></tr>
<tr><td>2</td><td>D</td><td colspan="2">Increased complexity requires a greater need for designer expertise. Designers should be allowed to modify the design problems in each subsystem or levels.</td></tr>
<tr><td>3</td><td>D</td><td colspan="2">Information should be sufficient to analyze each subsystem and coupling.</td></tr>
<tr><td colspan="4">Computational Cost Management</td></tr>
<tr><td>4</td><td>D</td><td colspan="2">Efficient solution search methods should be implemented.</td></tr>
</table>

5	D	Surrogate models should be employed to replace the computationally intensive original model.
6	W	Collaborative design process will improve the efficiency.
Uncertainty Management		
7	D	Uncertainty in control factors and noise factors should be managed.
8	D	Uncertainty in individual subsystem model should be considered – model should be accurate enough.
9	D	Uncertainty propagation throughout the information flow in the system chains should be managed.
10	D	Surrogate model used in design process should be accurate enough especially when model is nonlinear.

Complexity management, computational cost management and uncertainty management are three primary challenges in complex systems design. In order to keep the cost of design within an acceptable range, it is quite important to reduce the complexity, although problems are becoming more complex. Therefore, it is necessary to accurately abstract design problems and eliminate all trivial variables or factors. Designers should also be provided with freedom to modify the design problem based on expertise. Information of the system should also be sufficient, so that all important couplings in the system can be recognized and modeled. Computational cost is another challenge in complex system design. Efficient design exploration method is necessary to manage the increased complexity due to computationally intensive subsystem models and increased number of design variables. Therefore, efficient surrogate meta-models and solution search methods are two ways to keep the computational cost of complex systems design within acceptable ranges. In addition, if a collaborative design process is available and designers and works in parallel, the efficiency of design process can be improved a lot. The third challenge is uncertainty management. Complex systems design includes all types of uncertainties, including the uncertainty in control factor and noise factor [11], model uncertainty [12] and uncertainty propagation throughout the model chains [13]. It is necessary for a robust design approach for complex systems to manage all kinds of uncertainties.

These challenges are addressed in this thesis by employing the design exploration method for adaptive design systems based on existing robust design method, the Inductive Design Exploration Method, and a model regression method, the local regression method. These methods are expressed in the research questions and hypotheses in Section 1.3. In Section 1.2, the frame of reference for this method is established by discussing existing robust design approaches and current popular meta-modeling techniques.

1.2 FRAME OF REFERENCE

In Section 1.2, the frame of reference for this thesis is presented with a discussion of robust design and meta-modeling techniques. More details regarding each of these topics are presented in a literature review in Chapter 2.

1.2.1 Robust Design

Robust design is the practice of improving the quality of products by reducing sensitivity to noise factors, including uncertainty. When products are robust, performance levels remain stable despite the presence of noise factors [14, 15]. A robust solution may have lower performance levels than an optimum solution in the absence of variation; however, a robust solution produces predictably satisfactory results in the presence of variation. In complex systems design problems where the likelihood of uncertainty introduction and propagation is high, robust solutions are often favored.

The concept of designing for robustness was made popular by Taguchi [14]. Taguchi recognized that some noise factors could not be controlled; therefore, designs should be robust to these uncontrollable variations. Rather than increase the cost of a product by trying to eliminate noise factors, Taguchi proposed to minimize the variance of performance as well as bringing the mean on target. Uncertainty in complex systems design problems arises from noise factors, uncertain control factors, uncertain system models, and propagated process chain uncertainty.

The concepts of robust design proposed by Taguchi have been adapted to a robust design method for complex systems, the Inductive Design Exploration Method (IDEM) [4]. In IDEM robust solutions are selected by minimizing response variation while maximizing distance to design variable bounds. The IDEM provides designers with large design freedom in each stage so that designers do not need to worry about the uncertainty influence in the design process. In addition, the IDEM also makes collaborative design process possible. In the IDEM, designers are able to work on different subsystems design problems in parallel. However, IDEM has serious limitations which constrain its usage. The inefficient solution search process and high computational cost make it difficult to solve complex systems with increased number of design variables. Therefore, there is a possibility to modify the IDEM in order to improve the solution search efficiency while keep its advantages in uncertainty management. A formal review of robust design is presented in Chapter 2.

1.2.2 Meta-modeling Techniques

Simulation models are usually the only approach to obtaining a design solution in the design of complex systems. If the simulation models are computationally expensive, then the design process may rely on a mathematical model surrogate of system performance, to approximate the relationship between the system performance and design parameters, which is simply called metamodel. In systems design, it is quite important to implement the metamodeling techniques to reduce the computational cost.

One goal in this thesis is to introduce a meta-modeling method which can easily and more accurately fit nonlinear data compared to two currently popular statistical methods, response surface model and kriging model. The response surface model is one of the most popular statistical methods in the engineering design. Although it is easy to use, large errors may happen when it is implemented to fit nonlinear data. Part of "model parameter uncertainty" does come from the inaccurate simulation model. Kriging has better strength in interpolating responses of nonlinear data set. However, it is an interpolation method instead of a regression method. If there is noisy data existing, the response predictions will be seriously influenced. Therefore, it is necessary to explore an alternative statistical method to accurate fit nonlinear data in the system design. Different metamodeling techniques are studied and their advantages and disadvantages are compared in Chapter 2. In Chapter 3, local regression method is introduced to address the limitation of response surface model in fitting nonlinear data. When solving the example problems in Chapter 5, the local regression method is particularized for application.

The research gaps can be identified through the frame of reference in robust design approaches and statistical method used in the system design. In the next section, research questions and hypotheses are proposed to fill the research gaps.

1.3 RESEARCH FOCUS AND CONTRIBUTIONS

The primary and secondary research questions and hypothesis addressed in this thesis are given in Section 1.3. The research questions are formulated out of the need to develop a robust design approach for complex systems.

1.3.1 Research Questions and Hypotheses

The primary research question relates to the development of a robust design approach for the complex system to control the uncertainty in the adaptive design systems more efficiently. In the primary research hypothesis, it is proposed that a robust design approach modified from an existing multiscale robust design method, IDEM [4]. The primary research question and hypothesis are listed below.

Primary Research Question

How can we control the uncertainty in the adaptive design systems efficiently?

Primary Research Hypothesis

The uncertainty in the adaptive design systems can be efficiently by the design exploration method for adaptive design systems (DEM-ADS) with an inverse design exploration modified from the Inductive Design Exploration Method (IDEM).

The secondary research questions relate to the accuracy improvement of simplification of the complicated and nonlinear models. The secondary research question and hypothesis are listed below.

Secondary Research Question

How can the accuracy of surrogate models for computationally intensive and nonlinear simulation models be improved?

Secondary Research Hypothesis

The surrogate model for computationally intensive and nonlinear simulation models can be improved by the introduction of the local regression model into the design process.

Each of the research questions are addressed in specific chapters of thesis as outlined in Table 1. 2. The verification and validation of the robust design approach for complex systems is evaluated using the Validation Square Construct (see Section 1.4).

Table 1. 2 - Relevance of Thesis Chapters and Sections to Research Questions and Hypotheses

Relevant Chapters:	Chapter 2			Chapter 3				Chapter 4			Chapter 5			
Research Questions:	2.1	2.2	2.3	3.1	3.2	3.3	3.4	4.1	4.2	4.3	5.1	5.2	5.3	5.4
Primary	X		X	X	X		X	X	X	X	X	X	X	X
Secondary		X		X		X					X	X		

1.3.2 Research Contributions

The main contributions presented in this thesis are the development of a design exploration method to solve the adaptive design systems problem more accurately and efficiently. The research contributions are realized in addressing the primary and secondary research questions. Details regarding research contributions in this thesis are presented in Section 1.3.2 and analyzed in Section 6.1.

Robust Design Exploration Method for Adaptive design systems

The robust design exploration method for adaptive design systems is introduced in Chapter 3. This robust design method is developed based on the existing multiscale robust design method, the Inductive Design Exploration Method, and supposed to improve the solution search efficiency using efficient solution search methods instead of discrete exploration in the whole design space. The proposed method is a contribution to the field of engineering design because it provides designers with the possibility to solve more complex robust design problems with less computational cost.

Local Regression Method in Engineering Design

In Chapter 3, the local regression method is introduced. The local regression method is popular in the social survey and economic analysis. With the special feature to fit nonlinear data, it is useful to implement in the engineering design with highly nonlinear models. The local regression method is a contribution to the field of engineering design because it does provide designers with an alternative when dealing with complex simulations and it is also a way to reduce the uncertainty existing in the surrogate model used in design process.

Photonic Crystal Coupler and Waveguide Design

The motivating example in this thesis is the photonic crystal coupler and waveguide robust design. It is the particularization and application of the robust design approach for complex systems introduced in this thesis. The photonic crystal theoretical supports and the coupler and waveguide simulation models are provided by Dr. Vivek Krishnamurthy and Dr. Benjamin Klein in Electrical and Computer Engineering Department at Georgia Tech. It is a contribution to the photonic crystal design because it provides the designers a systematic design approach to deal with various uncertainty existing in the photonic crystal design.

1.4 METHOD VALIDATION STRATEGY – THE VALIDATION SQUARE

In this thesis, the verification and validation of the multilevel design template is assessed using the Validation Square construct. The Validation Square is a tool used to ease the leap of faith required to move from theory to practice in engineering design methodology. The progression of building confidence in the usefulness of the method based on the Validation Square is broken into four stages and is shown in Figure 1. 4 [6]. A review of method validation using the Validation Square is presented in Section 1.4. In Section 1.4.1, an overview of method validation is presented, and in Section 1.4.2, a strategy for validation and verification of this thesis is presented.

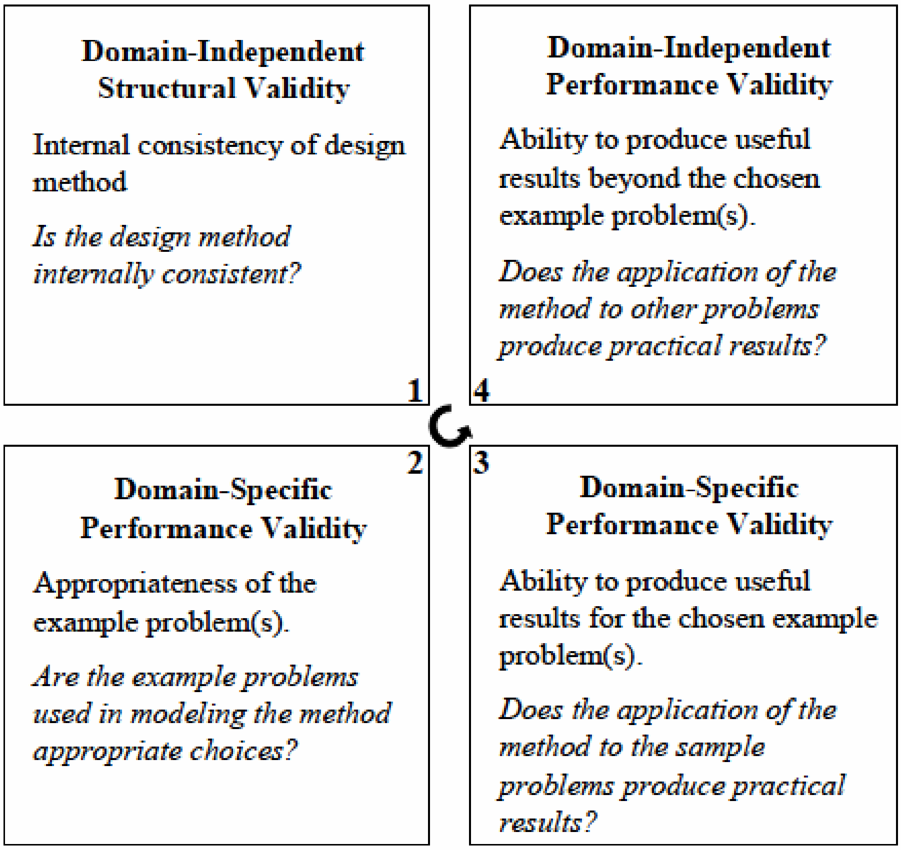


Figure 1. 4 - Validation square construct [7]

1.4.1 Validating Design Methods

Section 1.4.1 on method validation using and the Validation Square is leveraged with minor modification from the Ph.D. dissertation of Carolyn Conner Seepersad[6].

Validation—justification of knowledge claims, in a modeling context—of engineering research has typically been anchored in formal, rigorous, quantitative validation based on logical induction and/or deduction. As long as engineering design is based primarily on mathematical modeling, this approach works well. Engineering design methods, however, rely on subjective statements as well as mathematical modeling; thus, validation solely by means of logical induction or deduction is problematic. Pedersen and coauthors and Seepersad and coauthors propose an alternative approach to validation of engineering design based on a relativistic notion of epistemology in which “knowledge validation becomes a process of building confidence in its usefulness with respect to a purpose.”

The Validation Square is a framework for validating design methods in which the ‘usefulness’ of a design method is associated with whether the method provides design solutions correctly (structure validity) and whether it provides correct design solutions (performance validity). Additionally, the validity of the method itself (domain independent) and the method applied to example problems (domain-specific) is addressed. This process of validation is represented graphically in Figure 1. 5.

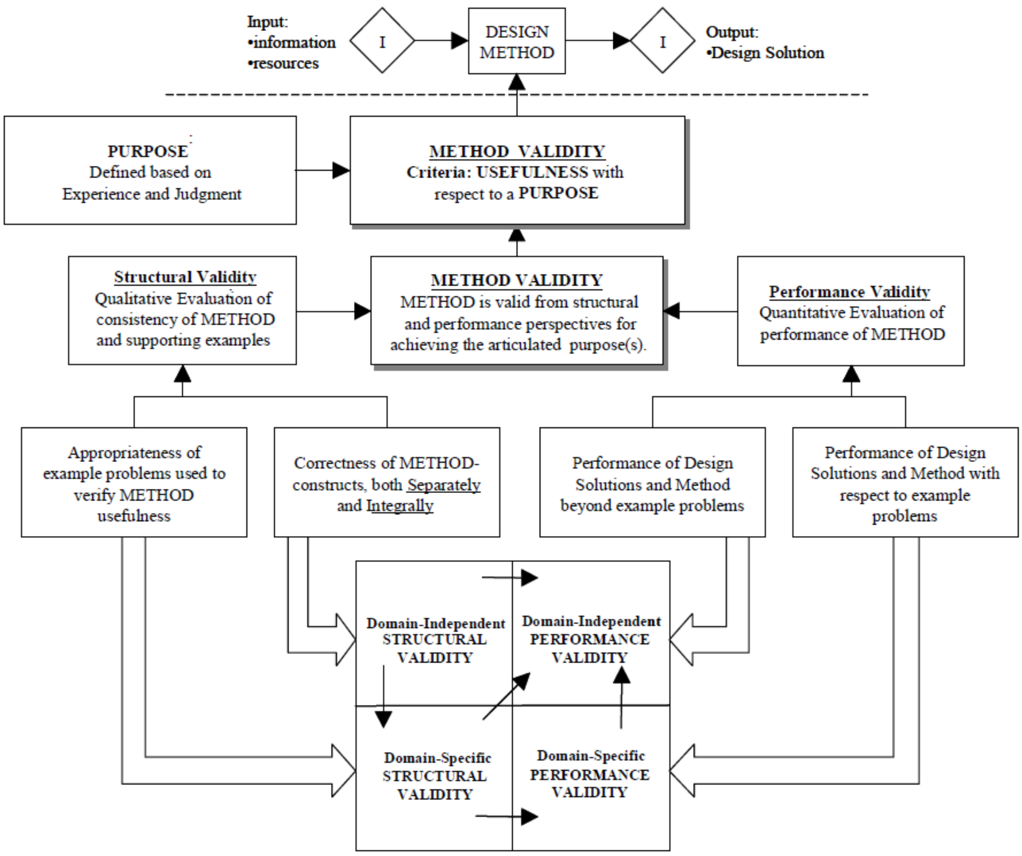


Figure 1. 5 - Design method validation: a process of building confidence in usefulness with respect to a purpose [6]

With respect to the quadrants of the Validation Square, domain-independent structure validity involves accepting the individual constructs constituting a method as well as the internal consistency of the assembly of constructs to form an overall method. Domain specific structure validity includes building confidence in the appropriateness of the example problems chosen for illustrating and verifying the performance of the design method. Domain-specific performance validity includes building confidence in the usefulness of a method using example problems. Domain-independent performance validity involves building confidence in the generality of the method and accepting that the method is useful beyond the example problems.

How can this validation framework be implemented in a thesis?

- Establishing *domain-independent structural validity* involves searching and referencing the literature related to each of the parent constructs utilized in the design method. In addition, flow charts are often useful for checking the internal consistency of the design method by verifying that there is adequate input for each step and that adequate output is provided for the next step. A list of criteria may be useful for establishing and comparing the domain-independent structural validity of methods and constructs with respect to a set of explicit, favorable properties.

- Establishing *domain-specific structural validity* consists of documenting that the example problems are similar to the problems for which the methods/constructs are generally accepted, that the example problems represent actual problems for which the method is intended, and that the data associated with the example problems can be used to support a conclusion.

- *Domain-specific performance validity* can be established by using representative example problems to evaluate the outcome of the design method in terms of its usefulness. Metrics for usefulness should be related to the degree to which the method's purpose has been achieved (e.g., reduced cost, reduced time, improved quality). It is also important to establish that the resulting usefulness is, in fact, a result of applying the method. For example, solutions obtained with and without the construct/method can be compared and/or the contribution of each element of the method can be evaluated in turn. An important part of domain-specific performance validity is empirical verification of data used to support domain-specific performance validation. Empirical verification can be established by demonstrating the accuracy and internal consistency of the data. For example, in optimization exercises, multiple starting points, active constraints and goals, and convergence can be documented to verify that the solution is stationary and robust. For any engineering model it is important to verify that data obtained from the model represents aspects of the real world that are relevant to the hypotheses in question. The model should react to inputs in an expected manner or in the same way that an actual system would react.

- *Domain-independent performance validity* can be established by showing that the method/construct is useful beyond the example problem(s). This may involve showing that the problems are representative of a general class of problems and that the method is useful for these problems; from this, the general usefulness of the method can be inferred.

1.4.2 Thesis Validation Strategy

In Table 1. 3 and Figure 1. 6, an outline of the validation strategy for this thesis is presented. It is arranged according to the quadrants in the Validation Square, and references are included for chapters in which method validation is documented.

Table 1. 3 - Validation strategy implemented in this thesis

Domain-Independent Structural Validity • Critically review the relevant literature and identify research opportunities. (Section 2.1, 2.2, 2.3) • Justify that two hypotheses are logically formulated to appropriate cover the research opportunities. (Section 2.4) • Discuss the developed design exploration method for adaptive design systems and local regression method is well constructed to instantiate the hypotheses in intellectual and methodological aspects. (Section 3.5) • Discuss the internal consistency of the developed robust design exploration method for complex adaptive design systems (Section 3.5).
Domain-Specific Structural Validity • Discuss the challenging aspects of the example, the simulation-based MESMs design, for the robust design exploration method for complex adaptive design systems and argue that the aspects are appropriate to test the primary hypothesis. (Section 4.1, Section 4.4) • Discuss the challenging aspects of the comprehensive example, the photonic crystal coupler and waveguide design, for the robust design exploration method for complex adaptive design systems and local regression method, and argue that the aspects are appropriate to test the primary and secondary hypothesis. (Section 5.1, 5.5) • Document the result data are appropriate for testing the hypotheses. (Section 5.5)
Domain-Specific Performance Validity • Validate the primary hypothesis based on the results obtained in the simulation-based MESMs design problem. (Section 4.4) • Validate the primary hypothesis and secondary hypothesis based on the obtained

results in the photonic crystal coupler and waveguide design problem. (Section 55.)
Domain-Independent Performance Validity • Discuss that the hypotheses in this thesis are also valid for general complex system design. (Section 6.1)

As shown in Figure 1. 6, each chapter in this thesis brings contributions in the Validation Square to validate the hypotheses proposed in this thesis. In the first quadrant of the Validation Square, Domain-independent Structural Validity, the appropriateness of the hypotheses is justified to cover the research questions. In Chapter 2, the research gaps and opportunities are identified, and key elements in the proposed methods are found in the literature review, which are implemented in the proposed methods to address the research gaps. In Chapter 3, the proposed methods for primary hypothesis and secondary hypothesis are introduced. The internal consistency, strength and limitations of the proposed methods are examined. Chapter 2 and Chapter 3 make the Domain-independent Structural Validity complete. In the second quadrant of the Validation Square, Domain-specific Structural Validity, the appropriateness of the examples is justified for the validations of the hypotheses. The MESMs design problem is implemented to show the advantage of DEM-ADS in solution search efficiency; the PCCW design problem is used to show the better efficiency in solution search of DEM-ADS and the ability of the local regression method in creating more accurate models than response surface models. In the third quadrant, Domain-specific Performance Validity, it is illustrated how the results of the examples proposed to validate the hypotheses show the usefulness of the proposed methods in answering research questions and filling the research gaps in Chapter 4 and Chapter 5. In the fourth quadrant, Domain-independent Performance Validity, confidence is built in the generality and usefulness of the proposed methods beyond the specific examples. It is argued that the proposed methods can also be useful in other design examples when specific assumptions can be satisfied.

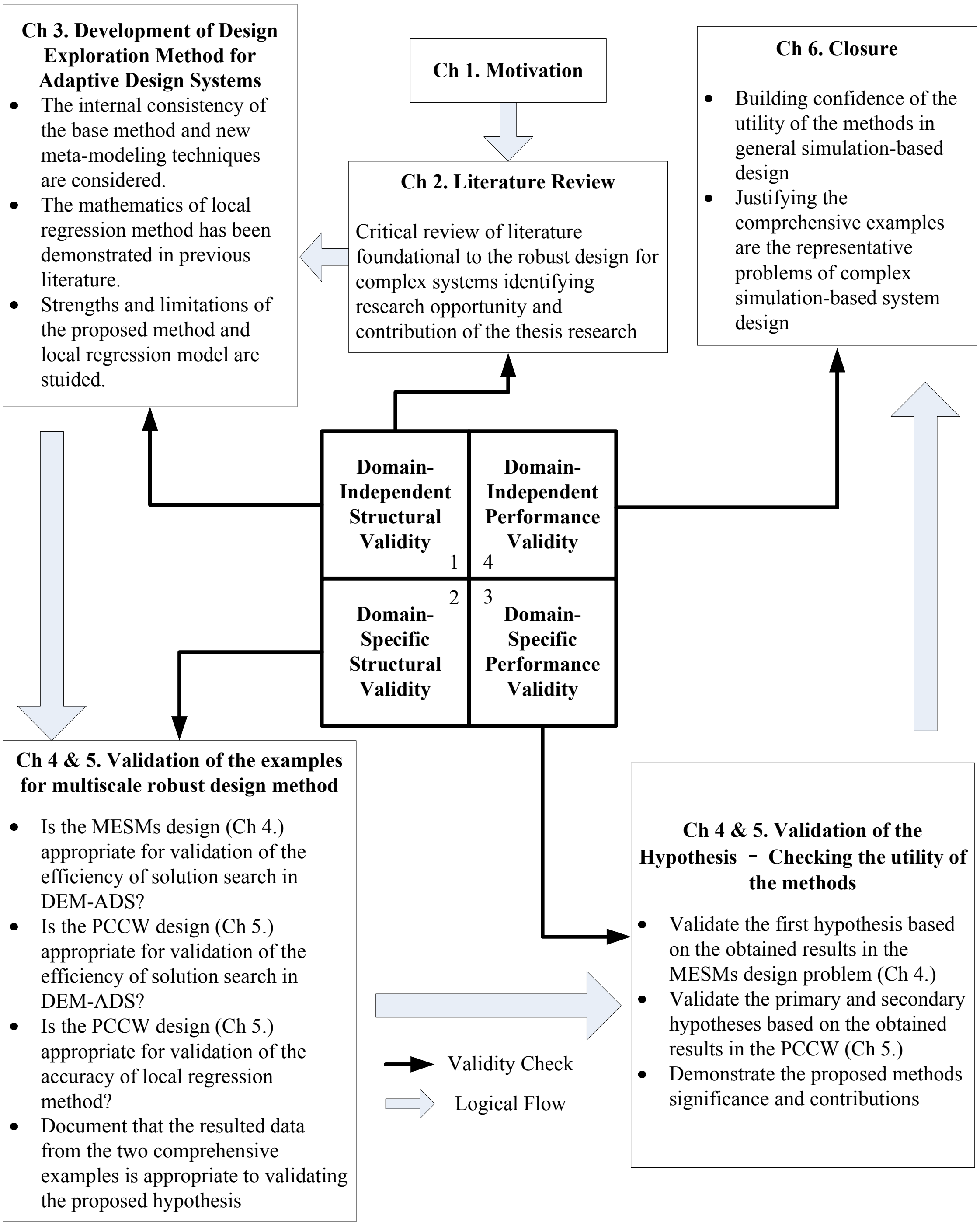


Figure 1. 6 - Validation strategy of the thesis

1.5 SYNOPSIS OF CHAPTER 1

The roadmap for this thesis is illustrated in Figure 1. 7. Chapter 1 provides the introduction and motivation for the thesis. It begins with the background and motivation section for systems design. In Section 1.2, the frame of reference for this thesis is established with a discussion of robust design approaches and metamodeling techniques. In Section 1.3, the research focus of this thesis is presented, including the primary and secondary research questions and hypothesis. Research contributions from this thesis are also discussed. The design method validation strategy used in this thesis is introduced at the end of Chapter 1.

In Chapter 2, the establishment of the motivation and frame of reference of the thesis with a review of relevant topics in design literature is discussed in order to identify areas of research opportunities. The identified research gaps in Chapter 2 directly correlate with the research questions presented in Chapter 1. In Chapter 3, the theoretical foundations of this thesis are developed with the creation and discussion of the design exploration method for adaptive design systems and local regression method. In Chapter 4 and Chapter 5, the proposed design approach is applied to two example problems. In Chapter 6 aspects of method validation presented throughout the thesis are brought together with a thorough assessment of the validity of the design exploration method for adaptive design systems. Chapter 6 also contains the research contributions of this thesis and opportunities for future research.

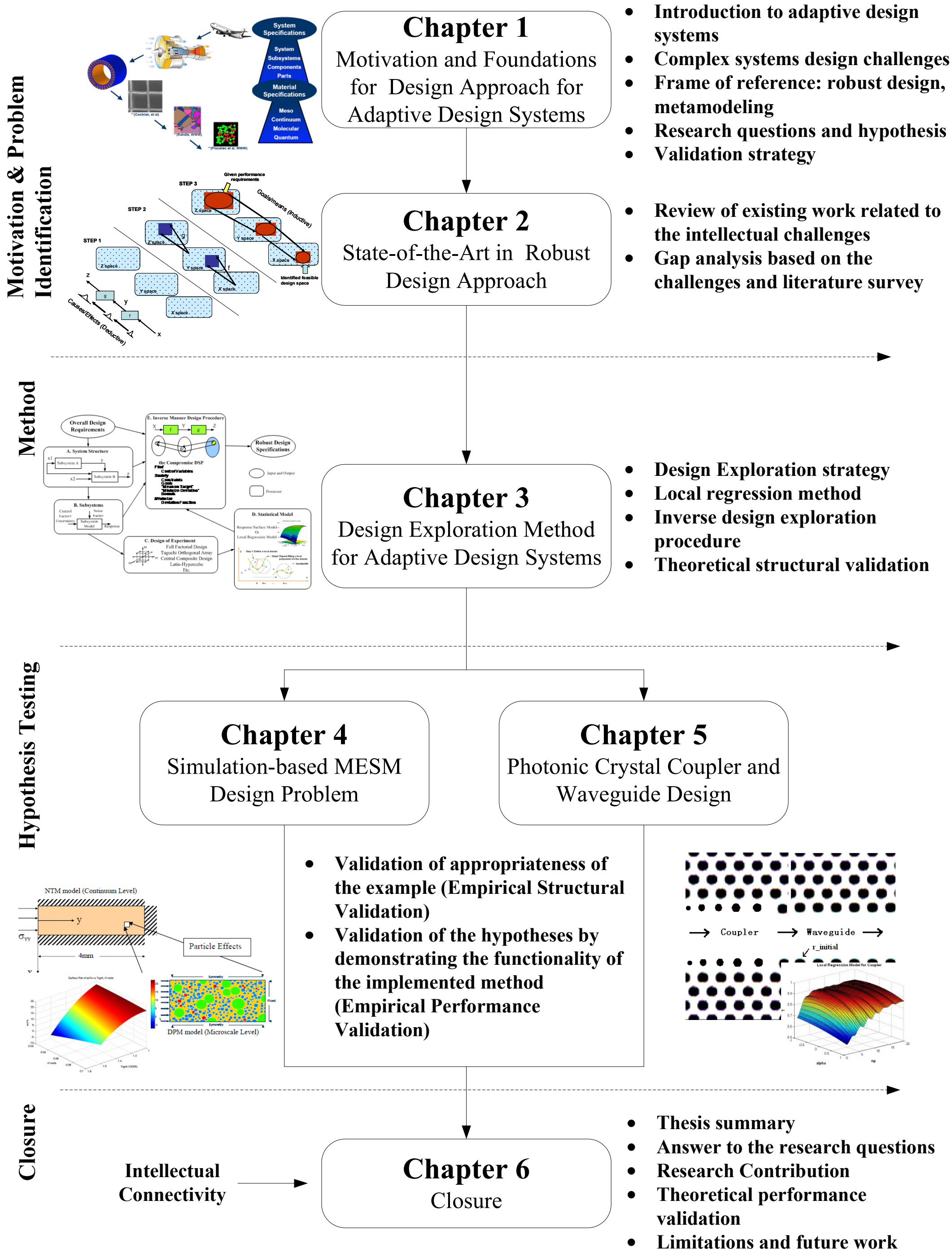


Figure 1. 7 - A roadmap for this thesis

CHAPTER 2
REVIEW OF LITERATURE AND IDENTIFICATION OF RESEARCH GAPS

In Chapter 2, key concepts of robust design for complex systems are presented. As illustrated in Figure 2. 1, the role of this chapter within the thesis is to introduce the methods and constructs necessary for the design exploration method for adaptive design systems. Theoretical structural validation is begun in this chapter by reviewing, referencing, and discussing the literature relevant to each of the constructs employed in this thesis. To begin, topics relating to different robust design approaches are discussed. Uncertainty classification and previously developed robust design methods are presented. Then, the meta-modeling techniques and solution search methods are studied. Each of these components is critically reviewed. Strengths, weaknesses, and accepted domains of application are discussed, as required for theoretical structural validation. At the end of Chapter 2, the research gap in developing robust design for complex systems is identified, which is the motivation for formulating the primary and secondary research questions.

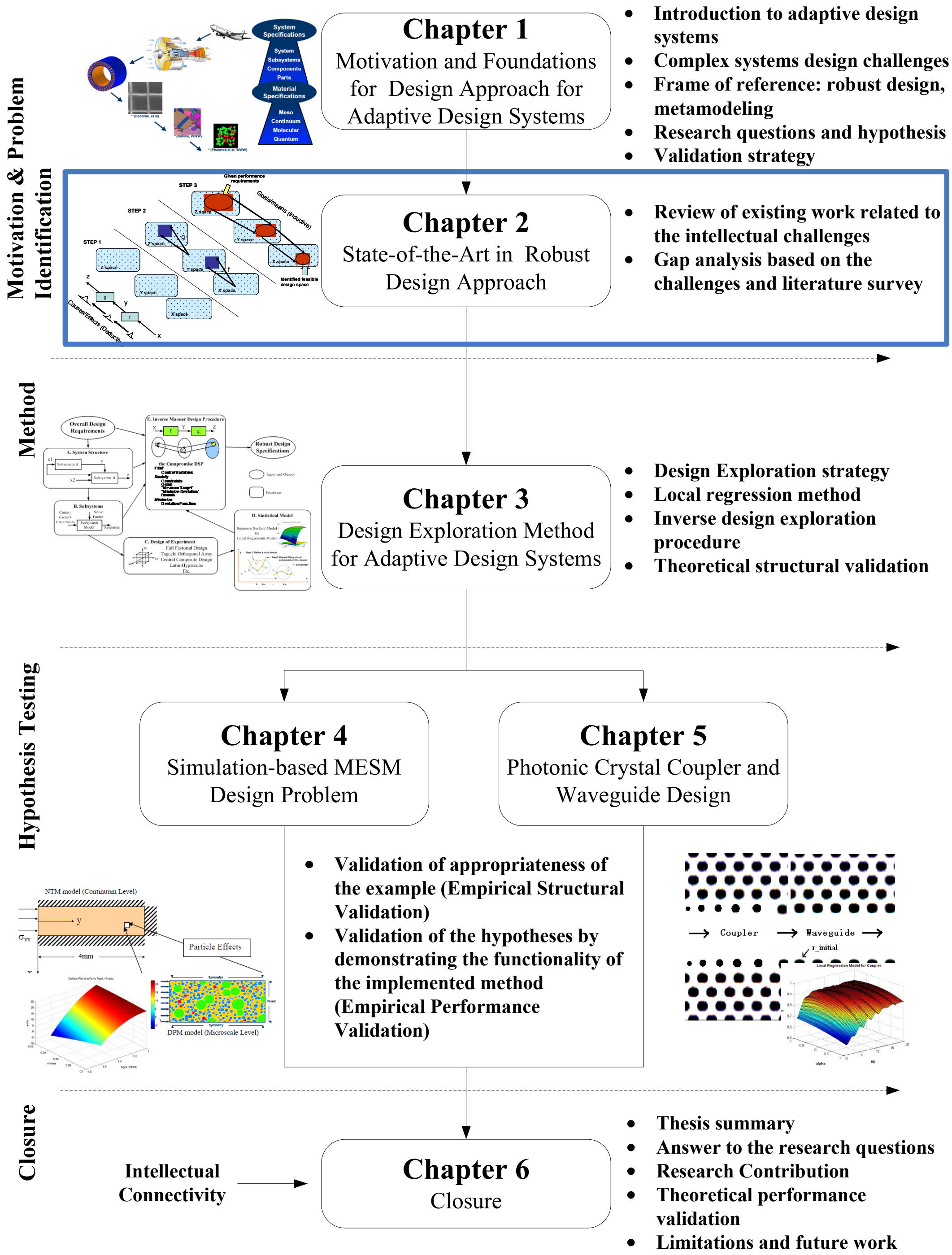


Figure 2. 1 - A roadmap of thesis

2.1 ROBUST DESIGN METHOD UNDER UNCERTAINTY

One important challenge in systems design is how to manage uncertainty efficient in the system design, because uncertainty usually leads to a wrong decision in system design, as discussed in Chapter 1. Eliminating uncertainties may be one possible solution to make the right decision, but it is almost impossible to eliminate all uncertainties in complex systems. Therefore, robust design was proposed to design systems insensitive to those uncertainties without eliminating uncertainties a few decades ago. Many new robust design techniques make possible the uncertainty management in complex systems design. In the following section, a discussion on different types of robust design methods for uncertainty management in a design process is presented. Information in Section 2.1.1 to Section 2.1.3 are leveraged from the Ph.D. dissertation of Hae-jin Choi [4].

2.1.1 Definition of Robust Design

The best way for making the right decision is eliminating those uncertainties; however, eliminating uncertainty in a model is often practically infeasible and reducing uncertainty may be costly and time-consuming. Robust design is a method for improving the quality of products and processes by reducing their sensitivity to variation, thereby reducing the effects of variability without removing its sources [14, 15]. There are three kinds of robust design. Type I robust design is used to identify control factor values that satisfy a set of performance requirement targets despite variations in noise factors. Type II robust design is used to identify control factor values that satisfy a set of performance requirement targets despite variation in control factors themselves. Type III robust design is used to identify adjustable ranges for control factors that satisfy a set of performance requirement targets and are insensitive to variability within the system model. In addition, three types of robust design may be combined to deal with uncertainty propagation throughout the design chain. In the next several sections, each type of robust design is studied in order to identify the research possibility to improve robust design technique for complex systems design.

2.1.2 Taguchi Method – Type I Robust Design

One of the main forms of uncertainty in a system model is uncertainty in uncontrollable independent system parameters, which are known as “noise factors”. Noise factors are in parametric form and may be quantified and characterized as continuous numbers with or without uncertainty information. In order to design a system robust to the uncertainty in noise factors, Type I robust design was proposed by Taguchi [4].

Type I robust design is to identify system values that satisfy a set of performance requirement targets despite variation in noise factors. Taguchi proposed a signal-to-noise ratio for measuring sensitivity analysis of responses to variation of noise factors instead of a statistical test, such as F-test, using a traditional approach, ANOVA. Based on an average response plot (mean of response variation) and signal-to-noise ratio (deviation of responses), designers select the best combinations of the level of each control factor. Taguchi method is practical, intuitive and relatively simple. This method has also been widely applied to the industrial problems and achieved successful outcomes.

Although Taguchi’s robust design principles are advocated widely in both industrial and academic settings, his statistical techniques, including orthogonal arrays and signal-to-noise ratios, have been criticized extensively. The orthogonal array of the experimental design in Taguchi’s robust design has been criticized as inefficient and costly because it requires an unnecessarily large number of experiments. The signal-to-noise ratio for capturing response variation has been criticized on the grounds that designers could miss useful information because the signal-to-noise ratio confounds both the mean and variance of response in its formulation.

The Taguchi method has been criticized and many alternative approaches have been developed based on this method. His philosophy of robust design has been widely adapted in many applications in both academia and industry. Therefore, it is a milestone as a design philosophy, achieving not only good performance but also insensitivity to the noise influence.

2.1.3 The Robust Concept Exploration Method Type I and II Robust Design

The second form of uncertainty in a system model is uncertainty in design variables, which are known as "control factors". Similar to noise factors, control factors may be also measured and characterized as continuous numbers with or without probability distribution. Designers can determine the means of control factors, but the deviations of control factors may not be controllable. Therefore, control factors should be characterized in a manner similar to noise factors. In order to design a system robust to the uncertainty in control factors, Type II robust design was proposed by Chen and coauthors [16] as shown in Figure 2. 2. When the variation in a control factor exists, the optimizing solution produces larger variance in deviation in a response than the robust solution does in some cases. Therefore, they suggest finding a flat region rather than an optimal point, at which system's performance will be degraded significantly at slight deviation from the optimal decision points.

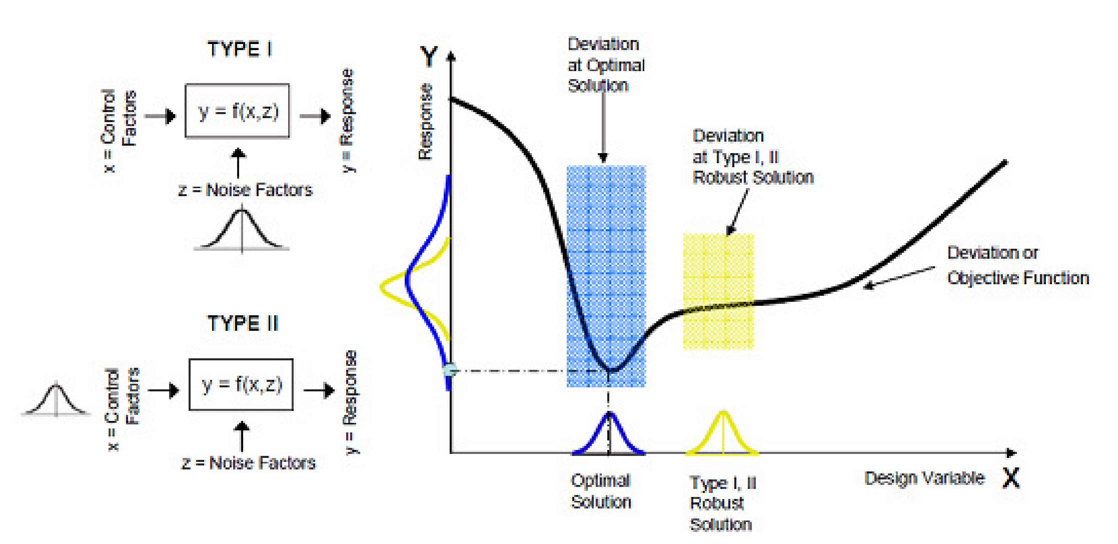


Figure 2. 2 - Robust design for variations in noise factors and control factors. Modified from [4]

A method combining Type I and Type II robust design in the early stages of product development, namely, the Robust Concept Exploration Method (RCEM) has been developed [16]. It is a domain independent method for generating robust, multidisciplinary satisficing design solutions. RCEM facilitates replacement of computationally expensive analysis software with fast, efficient, surrogate models. Therefore, rapid, efficient exploration of complex systems is made possible by integrating statistical experimentation and metamodeling. This method is useful for solving complex problems, which is very difficult to find a solution due to the highly non-convex design space and problem formulation. The computational infrastructure for the RCEM is illustrated in Figure 2. 3.

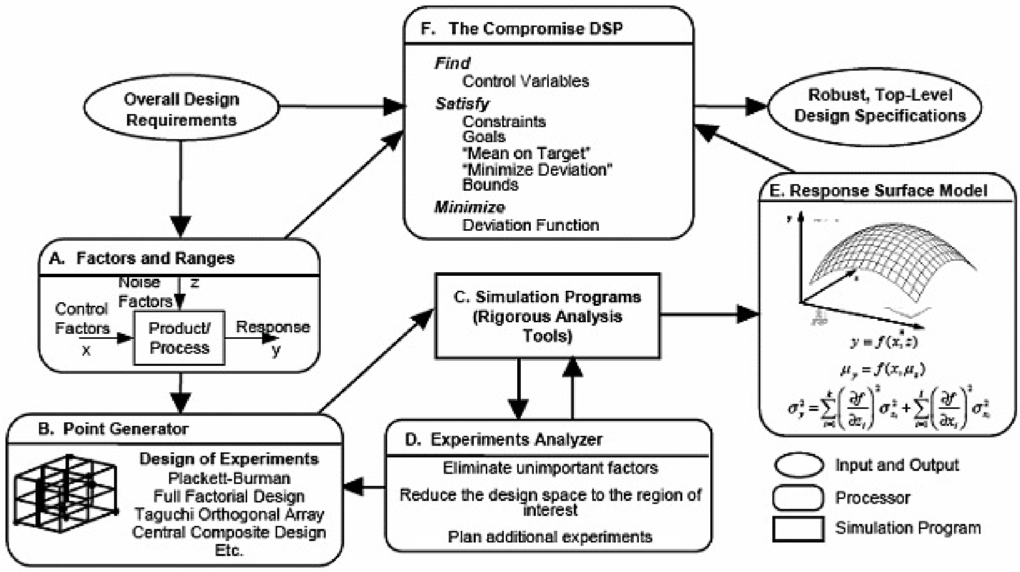


Figure 2. 3 - Computing Infrastructure for the Robust Concept Exploration Method [16]

Specifically, as illustrated in Figure 2. 3, the Robust Concept Exploration Method (RCEM), consists of such components as statistical experimentation and approximate models, robust design techniques, multidisciplinary analyses, and multiobjective decisions modeled with the compromise Decision Support Problems (cDSPs) for determining the values of design variables that satisfy a set of constraints and balance a set of conflicting goals, including bringing the mean on target and minimizing variation associated with each performance parameter.

Central to the RCEM is the cDSP. The cDSP is the mathematical construct through which the conflicting goals in robust design are modeled. The cDSP provides a mean for solving multi-objective and non-linear design problems [17]. Mathematically, the cDSP is a domain-independent, multi-objective decision model which is a hybrid formulation based on Mathematical Programming and Goal Programming [18]. It is used to determine the values of the design variables, which satisfy a set of constraints and bounds while achieving as closely as possible a set of conflicting goals. Since an important aspect of design is to model and handle multiple trade-offs simultaneously; the compromise DSP is used to model such decisions [19]. In this paper, it is shown that the compromise DSP can be used as a foundational, mathematical construct for structuring the search for families of compromise solutions for complex design problems. The word formulation of the cDSP is as follows [20]:

Given: A feasible alternative, assumptions, parameter values and goals

Find: Values of independent system variables (they describe the physical attributes of an artifact) and deviation variables (they indicate the extent to which the goals are achieved.)

Satisfy: System constraints, system goals, and bounds on variables

Minimize: Deviation function that measures the deviation of the system performance from that implied by the set of goals and their associated priority levels or relative weights.

The system descriptors (system and deviation variables, system constraints, system goals, bounds, and the deviation function) are described in detail by Mistree, Hughes and Bras [18] and are not repeated here. In the compromise DSP, each of the goals Ai, has two associated deviation variables d_i^- and d_i^+ that indicate the extent of the deviation from the target. The product constraint $d_i^- \cdot d_i^+ = 0$ ensures that at least one of the deviation variables for a particular goal is always zero.

Sometimes, the goals are not equally important. In order to affect a solution on the basis of preference, the goals may be rank-ordered into priority levels. The designers rate certain product qualities higher or lower than other qualities. A designer may look for a solution that minimizes all the unwanted deviations from the desired qualities. The mathematical formulation of the cDSP is shown in Figure 2. 4.

GIVEN

An alternative to be improved through modification
Assumptions used to model the domain of interest
Tbe system parameters:

n	number of system variables
p+q	number of system constraints
p	equality constraints
q	inequality constraints
m	number of system goals
$C_i(\mathbf{X})$	Capability of the system
$D_i(\mathbf{X})$	Demand to the system
$g_i(\mathbf{X})$	System constraint function

$$g_i(\mathbf{X}) = C_i(\mathbf{X}) - D_i(\mathbf{X})$$

$f_k(d_i^+, d_i^-)$ Function of deviation variables to be minimized at priority level k the preemptive case

FIND

X_i	System Variables	i = 1,..., n
d_i^+, d_i^-	Deviation Variables	i = 1,..., m

SATISFY

System Constraints (linear, nonlinear)

$g_i(\mathbf{X}) = 0$ i = 1,..., p

$g_i(\mathbf{X}) \geq 0$ i = p+1,..., p+q

System Goals (linear, nonlinear)

$A_i(X) + d_i^- - d_i^+ = G_i$ i = 1,..., m

Bounds

$X_{i,\min} \leq X_i \leq X_{i,\max}$ i = 1,..., n

$d_i^+, d_i^- \geq 0$ i = 1,..., m

$d_i^+ \cdot d_i^- = 0$ i = 1,..., m

MINIMIZE

Deviation function: Archimedean formulation

$Z = \sum_i W_i \left(d_i^+, d_i^-\right)$ i = 1,..., m

Figure 2. 4 - Mathematical Formulation of the Compromise Decision Support Problem [18]

RCEM is a domain-independent approach for generating robust, multidisciplinary design solutions. Robust solutions to multifunctional design problems are preference-weighted trade-offs between expected performance and sensitivity of performance due to deviations in design or uncontrollable variables. These solutions may not be absolute optimal within the design space. By strategically employing experiment-based metamodels, some of the computational difficulties of performing probability-based robust design are alleviated. Moreover, RCEM is unique among the robust optimization methods because it employs the compromise Decision Support Problem to compromise the achievements of multiple goals by controlling deviation variables from the multiple targets.

Despite its advantages, the RCEM has limitations in its capabilities, especially in complex systems design. In the RCEM, the whole system is considered as a single design problem. Internal couplings are not taken into considerations. Therefore, this method may not be useful for collaborative design or large-scale design in which important decisions should be made between the single-level couplings between different subsystems and multi-level couplings between the subsystem and lower-level components. Moreover, the response variance analysis in the RCEM is based on an important assumption that the computational model is accurate. The response surface method used in the RCEM may not be appropriate for complex nonlinear models. Large errors may happen between actual value and prediction value. In order to address this limitations, kriging model was proposed to replace response surface model in the RCEM[21]. Although kriging is better at fitting nonlinear models than response surface, it also has several limitations, which are discussed in Section 2.2. Furthermore, the estimation of performance variation based on the employed mathematical techniques, such as first order Taylor series expansion, may be inaccurate when the variations in noise and control factors are large or the model is highly nonlinear. Last but not least, in the RCEM, the performance and performance variability are two design goals, and designers have to make trade-off between them. Usually, it is difficult to define the weights of these two goals.

For complex systems design, although the RCEM is limited, it does provide good computing infrastructure to solve the design problem, especially the idea of how to use meta-modeling techniques and the compromise Decision Support Problem to achieve the robust solution efficiently. It provides the opportunities to adapt this method to complex systems design.

2.1.4 RCEM-EMI – Type III Robust Design

The third factor for the uncertainty embedded in system functions is "model parameter uncertainty", which is due to a combination of limited data and nonparametric system noise. This is the typical type of uncertainty in materials design that employs computationally intensive models. The final factor for the uncertainty embedded in a system model is "model structural uncertainty" that is due to assumptions and idealization in a system. The uncertainty embedded in a system model cannot be managed by previous robust design approaches (Type I and Type II). In order to manage this uncertainty, a new type of robust design approach, called Type III robust design, is proposed. A visual representation of Type III robust design, compared to Type I and Type II robust design, is shown in Figure 2. 5.

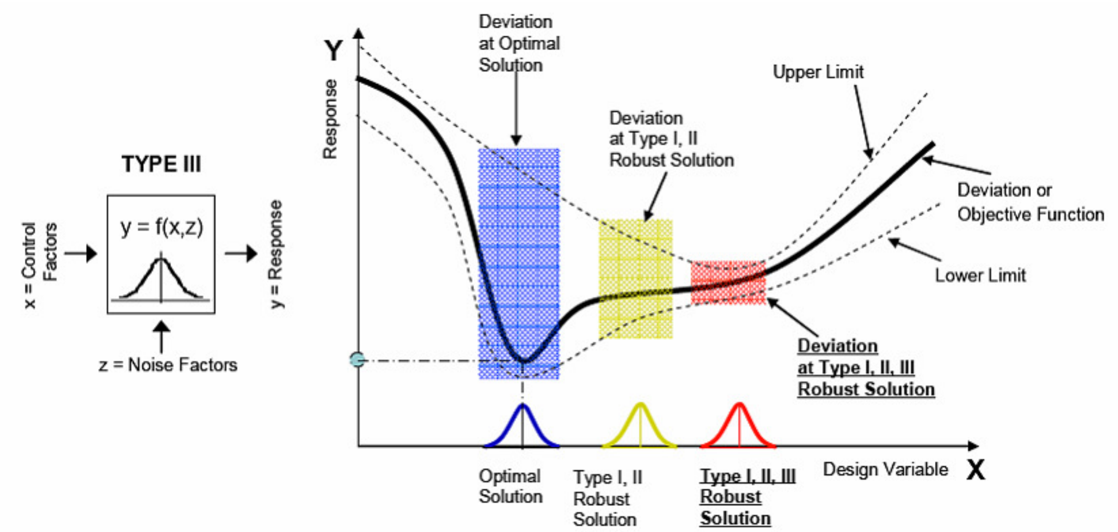


Figure 2. 5 - Type III robust design [4]

Type III robust design is to identify adjustable ranges for control factors that satisfy a set of performance requirement targets and/or performance requirement ranges and are insensitive to the variability within the model, as illustrated in Figure 2. 5. In the figure, the same objective function curve as in Figure 2. 2 is employed to show the differences among the optimal solution, Type I and II robust solution, and Type I, II and III robust solutions. A objective function which represents the system's response is illustrated as a solid curve. In addition, two dotted curves are added around the objective function, representing design requirement limits which are defined by design goals. Considering not only the objective function but also the two requirement limits, the optimal and Type I and II robust solution have larger deviations than the Type I, II and III robust solution.

Type III robust design becomes increasingly important since modern engineering systems are getting more complex and their behaviors are uncertain. Compared to Type I and II robust design, Type III robust design has not yet been studied rigorously in engineering systems design. The absence of the studies is due to ignorance about this uncertainty in most of the traditional engineering systems design problems or the difficulties in quantifying and incorporating this uncertainty into a design exploration process.

Du and coauthors proposed the extreme condition approach to deal with system uncertainty (Du, et al. 2000). Their approach considers both parameter and model uncertainty by deriving a range of system output based on extreme conditions and is developed to propagate the effect of uncertainties in order to enable designers to make reliable decisions. However, the disadvantages of this approach are also obvious. First, the computational efficiency of this approach is too poor to solve the large size of the problem since the Monte Carlo simulations are implemented to propagate the effect of uncertainties. Secondly, this approach also depends on the accuracy of the error model. The propagated integrated method may generate unsatisfactory result if the model greatly deviates from the real model or error model does not accurately describe the real situation. This disadvantage exactly prevents this approach from usage in the complex design problem or early design stage, in which huge amount of uncertainties exist, and it is hard to find an error model to accurately reflect the actual situation.

Derived from the extreme condition approach, system uncertainty analysis (SUA) and the concurrent subsystem uncertainty analysis (CSSUA) are introduced [22]. SUA and CSSUA are developed for improving the efficiency of uncertainty analysis with the feature of the multidisciplinary design optimization. Significant computational savings are achieved by employing Taylor expansion instead of Monte Carlo simulation. The assumption of these approaches is acceptable for two multidisciplinary robust design problems. If high accuracy is needed or more design subsystems are included, these approaches may not be efficient any more. These approaches are expected to be extremely computational expensive.

The Robust Concept Exploration Method with Error Margin Indices (RCEM-EMI) is proposed as a method for Type I, II and III robust design [4]. The overall procedure of the framework is shown in Figure 2. 6.

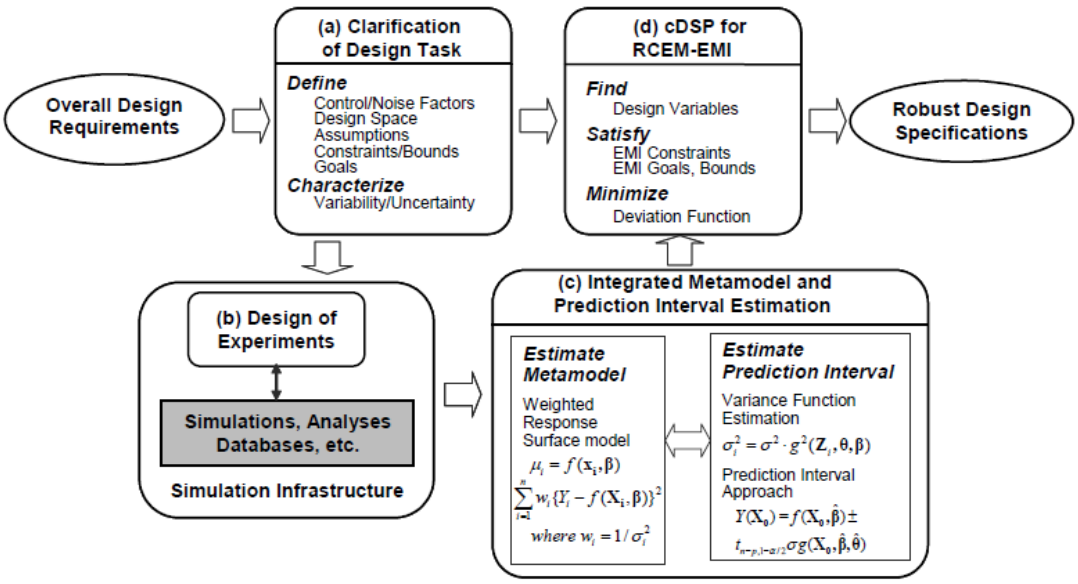


Figure 2. 6 - The RCEM-EMI construct [4]

The RCEM-EMI procedure consists of (a) clarification of the design task, (b) DOE and simulation, (c) integrated metamodel and prediction interval estimation, and (d) design space search using the cDSP for the RCEM-EMI. In the RCEM-EMI, the Error Margin

Indices (EMI) are metrics indicating the degree of reliability of a decision that satisfies system constraints and bounds [4]. The design procedure is to find ranged sets of design specifications that meet a range of system requirements based on the EMIs calculations. Unlike Type I and II robust design, in which only system response variations due to uncertainty from control factors and noise factors are considered, the RCEM includes the response variation due to the variability of the model itself and uncertainty bounds of models into the consideration. A case of two uncertainty bounds with a single design variable is illustrated in Figure 2. 7.

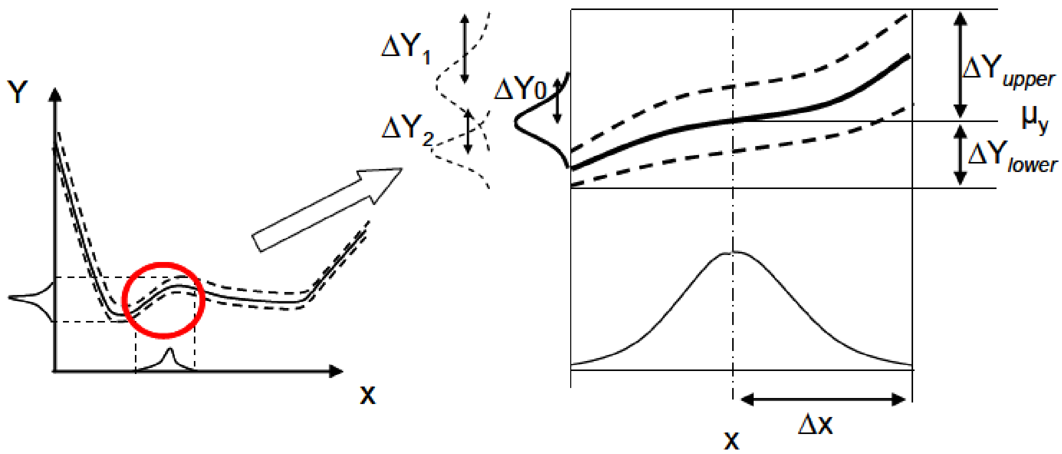


Figure 2. 7 - Formulation of uncertainty bounds due to variations in a design variable and a model [4]

The most probable model (e.g., a mean response model of a system) is shown in a solid curve with two uncertainty bounds (e.g., bounds on a prediction interval) shown as dotted curves. On the right hand side of the figure, the corresponding response variations of the system model and the uncertainty bounds within the interval of the design variable's variance are illustrated. The variation of the response in this case is influenced by not only the mean response but also the uncertainty bounds. The maximum and minimum response caused by variability in design variable sand models can be obtained from mean response model and uncertainty bound functions. The compromise Decision Support

Problem is then formulated to search the design specifications which can keep the maximum or minimum response far away from the boundary defined by design requirements [4]. The detailed calculation and introduction of EMI are discussed in Chapter 3.

When compared the RCEM-EMI and the RCEM, it is easy to realize that the RCEM-EMI is directly modified from RCEM, so that it also inherits the advantages of the RCEM. It is efficient for evaluating a family of designs, easy to understand and easy to compute, and incorporates multiple aspects in quality improvements [23]. In the RCEM-EMI, designers avoid the difficulties of trading off between performance and performance variability [4]. In the RCEM, the uncertainty from model is also taken into consideration. This method helps designers make a decision under system's random variability and/ or model parameter uncertainty (uncertainty from control factors and noise factors) in a model. It has also been shown that the design specifications identified by this method are more robust against variability that is difficult to parameterize, such as random material micro-structure change that causes large variations in system performance [4, 24].

Despite its advantages, the RCEM-EMI still has limitations, especially in the accuracy of metamodels. As same as the RCEM, the response surface method is employed to create surrogate models. The response surface method works especially poorly when fitting the data includes both highly nonlinear and linear parts. These kinds of models are very common in complex systems design.

The RCEM-EMI provides a good foundation for further development of the robust design method for complex systems. It provides a possibility to include EMIs calculations into the complex system design problem to achieve robust specifications.

2.1.5 IDEM – Robust Design for Complex Systems

The fourth type of uncertainty in a complex system is that generated in the design and analysis process chain, which, unlike the aforementioned uncertainties in a system model, arises from the complex design and analysis process chain. This type of uncertainty is often observed in multidisciplinary uncertain system design problems and includes errors in decisions made by other designers and accumulated errors (propagated uncertainty) by subsequent series of uncertain subsystem models. Typically, complex multidisciplinary system design requires multiple experts to collaborate to make decisions for designing a system. The outputs of other experts' decisions in a subsystem could be input parameters, constraints, or design spaces of other subsystems or systems design. In many cases, multiple subsystem designs even share common design variables. In these interactions in design activity, a subsystem design error can be propagated to another subsystem or system. Additionally, complex systems design tends to employ multiple analyses and simulations in series to predict system responses [7]. An example of uncertainty propagation through a model chain is illustrated in Figure 2. 8.

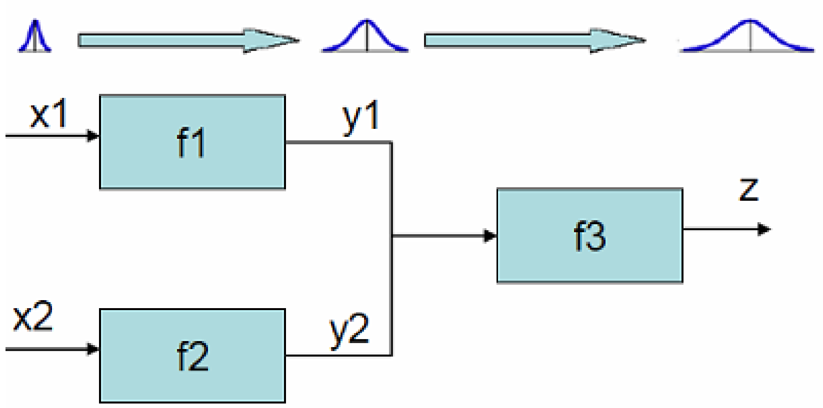


Figure 2. 8 - Uncertainty propagation through a design chain (modified from [4])

In this example, the parameter, x1, is an input to the subsystem model, f1; x1 has a variance associated with it. The y1 is the response from the model in which the input uncertainty is increased because of the combination of variance of x1 and errors in f1 model itself. Similar things happen in y2, which is the response of f2 with x2 as the input.

The same effect may be applied to model, f3. Variables, y1 and y2, are inputs with variances to f3. The response, z, includes increased uncertainty due to the combination of variances in y1 and y2 and the uncertainty in the model, f3. Therefore, uncertainty accumulates through multiple steps of a model chain and making the variance of the final response unexpectedly large. In order to deal with this kind of uncertainty, the robust design approach for complex systems is necessary.

The robust design approach for complex systems is to identify adjustable ranges of control factor (design variable) values under potential uncertainty and uncertainty propagation in a design and analysis process chain; account for uncertainty in downstream activities and uncertainty propagation. The Inductive Design Exploration Method (IDEM) [13] is proposed as a robust design approach for complex systems.

The assumption of IDEM is that the uncertainty which comes from the error of models and then is propagated during the design process can be reduced by keeping the design freedom as large as possible in each design stage. Therefore, IDEM does not provide any specific solutions, but a feasible design space. In this approach, the basic idea for finding ranged sets of robust solutions against the propagated uncertainty in a complex model chain is to pass down the feasible solution range in an inverse manner, from desired given final performance ranges to the design space, while the design freedom in each step is kept as large as possible. The design freedom in IDEM is defined as the ratio of the feasible ranges versus entire design space. For identifying feasible solution range, designers use only mathematical models for bottom-up calculation, not the materials models for the inverse calculation. Designers chose the solutions from this space according to their preferences or experience. The discrete exploration process is implemented in IDEM to explore the whole design space and check whether all individual design variables are able to create feasible performance. Since the discrete exploration process is quite computationally expensive, IDEM may not support the design problems with a large number of design variables. Therefore, an additional assumption of IDEM is that the design space is small enough to allow for an exhaustive search of all possible design combination. Moreover, due to the discretization of a design space, discretization errors are not avoidable when the algorithm is checking the feasibility of a mean performance based on discretized feasible and infeasible points.

The overall procedure for IDEM is illustrated in the Figure 2. 9.

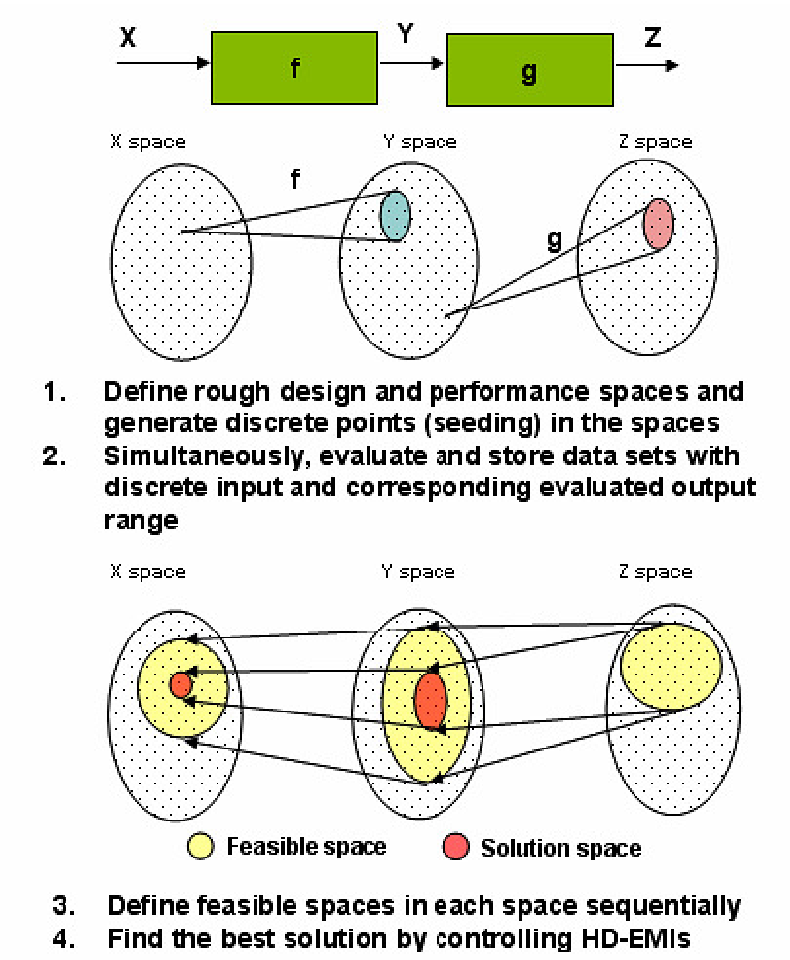


Figure 2. 9 - Solution search procedure for multi-level robust design [13]

The procedure includes the following steps [13]:

Step1: It is necessary to define the rough design space (x space in Figure 2. 9), the interdependent space (y space in Figure 2. 9), and the performance space (z spaces in Figure 2. 9). Discrete points are generated in each of these spaces.

Step2: The discrete points which are generated are evaluated based on the mapping models (model f and model g in Figure 2. 9) and the evaluated data sets which are composed of a discrete input point and output range are stored in a database.

These two steps combined are called the discrete function evaluation in the IDEM. Since it is common that an analysis chain includes shared variables with several models, the process for projecting shared input and output space is defined as the following:

- **Seeding**: Obtain all combinations of discrete input of associated input variables.
- **Splitting**: Group the combinations created in the 'Seeding' process by the input groups of evaluation functions.
- **Projecting**: Evaluate each sub-system function at the points in sub-seeds in order to get corresponding output ranges of each projection.
- **Merging**: Combine the multiple response ranges obtained from 'Projecting' process in order to formulate response ranges for each point in the original seeds.

Step3: Feasible regions in y and x spaces are sequentially identified by a metric for determining whether a discrete point from an input space maps to a feasible design solution in the output space, along with a given final performance range in z space. This metric is called Hyper-Dimensional Error Margin Index (HD-EMI). A visual and mathematical representation of HD-EMI is shown in Figure 2. 10.

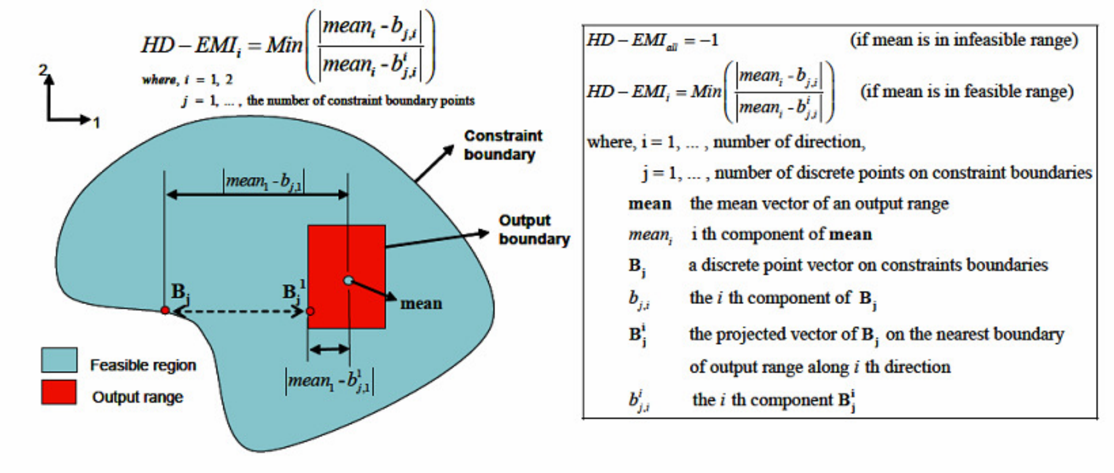


Figure 2. 10 - Calculation of HD-EMI [4]

HD-EMI is a measure of the distance of a design point from design space boundary divided by variation in system performance. As shown in Figure 2. 10, when HD-EMI increases, the output is farther away from the boundary and more likely to be satisfactory. Solution that is far from the boundary of the feasible design space will remain within the feasible design space in the presence of slightly variation. Therefore, in the IDEM, designers are interested in selecting ranges with high values of HD-EMI.

The Inductive Discrete Constraints Evaluation (IDCE) technique is implemented to sequentially find feasible ranges in all spaces, intermediate and design space based on the HD-EMIs. It is an inverse method for using the analysis process chain show in Figure 2. 11.

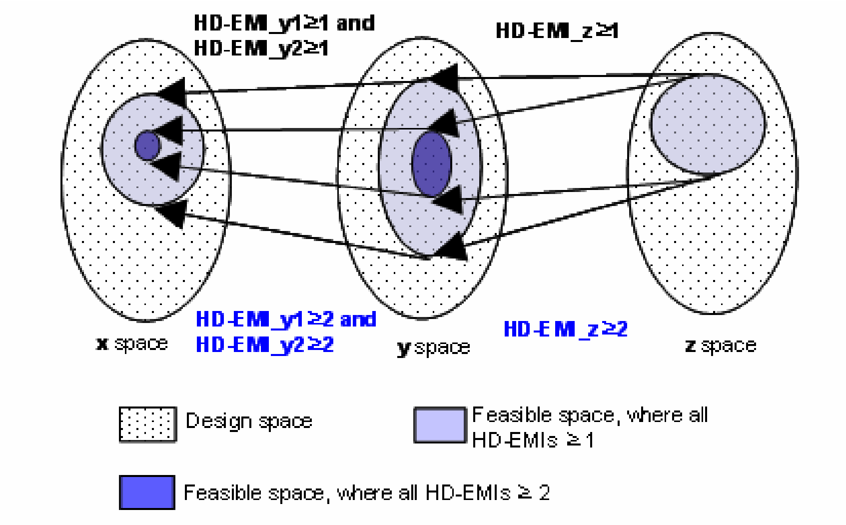


Figure 2. 11 - An example of the IDCE controlling HD-EMIs [4]

The evaluation procedure starts with an assumption that a required range of the final performance, z, is given as shown in the gray area in z-space in the figure. From the given required in z-space, a feasible range in y-space is obtained. In this step, first, feasible discrete points in y-space are found by evaluating whether the HD-EMI in z-space at each discrete point is greater than or equal to one. Second, exact border contours are identified between the feasible and infeasible discrete points in y-space, by identifying the discrete points in y-space in which the HD-EMIs in z-space are equal to one. Then, the next step is to find feasible regions in x-space based on the identified feasible region in y-space in the same way.

If there are multiple feasible discrete points in a design space, it means that designers have more room for tailoring design variables. In this case, the required HD-EMIs in the spaces of y and z can be increased, which may reduce the feasible ranges in x- and y-spaces, respectively. Designers need to make decisions to balance the number feasible discrete points in x- and y-space and the required HD-EMI value. In the IDEM, the compromise DSP is used to help designers determine the best solution.

IDEM is an excellent robust design approach for complex systems. In this method, designers are provided with sufficiently large design freedom in each step and the design freedom can also be changed by different required HD-EMI which can be defined by designers. The solution is also a ranged set of design specifications rather than single solutions, so that designers have more choices for adjusting the solutions to meet specific preferences or requirements. By keeping solutions far away from the design requirements boundary, the solutions obtained from IDEM are robust enough to different kinds of uncertainties. In addition, the IDEM also makes collaborative design possible in complex systems design problems. The design processes and function evaluations are decoupled and modularized. The collaborative design and parallel computing can be realized in a design problem employing the IDEM. When an analysis model in the system is changed, designers need to make decisions again in which function the changed model is involved, instead of evaluating all over subsystems. In IDEM, the input and output of analysis chain are also decoupled. Designers need only a data file that includes the mapping between input and output from a distributed model for later design exploration.

Despite its advantages, IDEM has limitations in its capabilities. One serious limitation of IDEM is its high computational cost. The discrete function evaluation process of the IDEM is obviously an exhaustive search method. All combinations of discrete inputs in the design space are evaluated. The computational cost depends on the discrete step size of each input variable. The IDEM may be computationally intensive for exploring a design space in which the number of design variables is large. It may not always be possible to reduce the number of design variable or employ parallel computation for function evaluation to reduce the computational cost. It may also increase the complexity of the design process if the parallel computing is used in the discrete exploration.

One purpose of this discrete function evaluation process is to explore the mapping relationship between the input and output of analysis, which is especially important in material design. As introduced in Section1.1, material design may be used to address the limitation that currently available materials may not achieve the design objectives. Therefore, designers have to tailor the materials in engineering design method and they do not have much information to predict whether the design objective is reasonable or not. In other words, the design objective may not be achievable within current material technology. The input and output of analysis is uncertain in material design. Therefore, it is necessary to discretely explore the whole design space to collect as much information as possible. The high computational cost of the discrete exploration in material design is worthwhile. However, in the adaptive design systems, such exploration may not be necessary. In adaptive design, designers have already obtained sufficient information about a simulation model so that the input and output analysis is known. Thus, discrete exploration is unnecessary in this kind of design problem.

The other purpose of the discrete function evaluation in IDEM is to provide designers with as large design freedom as possible. This purpose is based on an important assumption that such large design freedom in each design process is necessary due to the challenges of material design. For instance, major sources of uncertainty in processing, microstructure, model, etc., must be taken into consideration, since they can dominate the configuration of the design process. In addition, process capabilities may constrain specific microstructure obtained from the design process, and thermodynamics and kinetics considerations may also limit microstructure solutions. However, in this thesis, the design application is extended from material design to adaptive design systems. Such large freedom to address the material challenge may not be necessary for other design tasks. Instead, in my thesis, it is assumed that design freedom can be defined by designers according to different design environment throughout the top-down design tasks. Therefore, large design freedom may be always necessary in every design complex systems design problem.

In addition, it is also impossible to avoid discretization errors due to discrete point evaluations in the IDEM. Although an exact boundary generation technique for reducing the discretization errors is included in the IDEM, errors still exist in the constrains boundary representation and feasibility check of output means [4].

In the IDEM, the meta-modeling technique is the same as the RCEM-EMI. The response surface method is still the statistical method used to create surrogate models. Therefore, the limitations caused by response surface method are not solved in the IDEM.

A comparison of robust design methods according to the requirements of complex systems design is shown in Table 2. 1.

Table 2. 1 - Comparison of robust design methods according to the requirements of complex systems design

Requirements/Wishes for Systems Design	Different Types of Robust Design Methods			
	Type I	Type II	Type III	IDEM
Modify each subsystem design to reduce the complexity				X
Efficient solution search process	X	X	X	
Surrogate model should be employed	X	X	X	X
Surrogate nonlinear model should be accurate enough		X		
Collaborative design process				X
Uncertainty management in control factors and noise factors	X	X	X	X
Uncertainty management in system model			X	X
Uncertainty management in model chain				X

In Table 2. 1, it is shown that IDEM is an effective robust design method to be used in complex system design since it can satisfy most requirements, such as complexity management, collaborative design process support and uncertainty managements. However, IDEM cannot satisfy two requirements, that is, the efficient solution search and accurate surrogate model. Since most limitations of the IDEM arises from the discrete function evaluation process, thus, **is it possible to replace the discrete evaluation by more efficient solution search methods?** The other limitations of current robust design methods arise from the inaccurate surrogate nonlinear model. Thus, **is it possible to replace the response surface model by more accurate meta-modeling techniques for nonlinear models?** In order to answer these two questions, in the following sections, the literature about metamodeling techniques and solution search methods is studied to find the possibility to combine them with the IDEM in order satisfy all complex systems design requirements.

2.2 METAMODELING TECHNIQUES

In the design of complex systems, simulation models are usually the only approach to obtaining a design solution. The simulation models of the system performance depend on the knowledge of how systems perform. However, if the simulation models are computationally expensive, then the design process may rely on a metamodel, which is the mathematical model surrogate of system performance, to approximate the relationship between the system performance and design parameters. In metamodeling, there are basically two tasks that must be conducted: (i) select a set of sample points in the design parameter space; and (ii) fit statistical models to the sample points. Methods for the first task may be used to conduct sampling in general [25]. In this section, the review of metamodeling is presented and one of the research questions is proposed based on the statistical methods used in multiscale design.

2.2.1 Design of Experiments

Properly designed experiments are essential for effective computer utilization. The traditional approach in engineering is to vary one parameter at a time within a computer analysis code and observe the effects or to randomly assign different combinations of factor settings to be used as alternative parametric analyses for comparisons. Design of Experiments (DOE) represents techniques with which designers are able to reasonably select data points in the design space for fitting a model [26]. Several space filling experimental designs are discussed in the following.

Latin hypercube sampling (LHS)

LHS is a stratified sampling approach with the restriction that each of the input variables has all portions of its distribution represented by input values [27]. A sample of size Ns can be constructed by dividing the range of each input variable into Ns strata of equal marginal probability 1/Ns and sampling once from each stratum.

The LHS has the following advantages. First, it is computationally cheap to generate. Secondly, it can deal with a large number of runs and input variables. Thirdly, its sample mean has a smaller variance than the sample mean of a simply random sample.

Orthogonal Arrays (OA) Design

The experiment designs used by Taguchi, called orthogonal arrays, are most often simply fractional factorial designs in two or three levels. These arrays are constructed to reduce the number of design points necessary to evaluate the required effects.

There are mainly two limitations on the use of OA. First, this method lacks of flexibility. Given desired values for the number of rows, columns, levels, and strength, the OA may not exist. Secondly, OA designs projected onto the subspace spanned by the effective factors, most of which are influential design variables, can result in replication of points. This is undesirable for deterministic computer experiments where the bias of the proposed model is the main concern [28].

In this thesis, the design of experiments is not the focus. Research opportunities are explored in the statistical methods in next section.

2.2.2 Statistical Modeling

In statistical modeling, the objective is to estimate the relationship between a response variable, and several predictor variables. The response surface represents the true mean response. In the case of metamodeling, it is assumed that there is no error variability in the observed response values. Thus, the "mean" response coincides with the actual responses [26]. There are several statistical methods available for creating metamodels. In this thesis, only response surface model, kriging model and local regression model are studied in detail. The advantages and limitations of these methods are compared. The introduction of response surface model and kriging model are leveraged from Yao Lin and Timothy W. Simpson's Ph.D. dissertations [26, 29].

Response Surface Models

The general form of response surface (RS) models is a polynomial function of degree d. Since this is a linear model (in parameters), the usual linear model tools may be applied. Therefore, RS models are very easy to use. The drawback is that the rigid structure of a pre-selected polynomial model may not be flexible enough to represent the true response surface.

The general RS model can be expressed as the following.

$$\hat{y} = b_0 + \sum_j b_j x_j + \sum_j \sum_{k>j} b_{jk} x_j x_k + \sum_j b_{jj} x_j^2 + \sum_j \sum_{k>j} \sum_{l>k} b_{jkl} x_j x_k x_l + \ldots + \sum_j b_{j,j,\ldots,j} x_j^d \qquad (2.1)$$

Second-order RS models are widely used; however, they have a limited capability to model accurately non-linear functions of arbitrary shape. Higher-order response surfaces can be used to model non-linear design spaces, but instabilities may arise or it may be too difficult to take a sufficient number of sample points in order to estimate all of the coefficients in the polynomial equation, particularly in high dimensions.

The sequential response surface was proposed which uses move limits [30] or a trust region approach [31]. Other techniques recursively decompose the design space into subregions and fit each region with a separate model during design space refinement [32]. However, all of these sequential approaches are developed for single objective problems. Since many engineering design problems are multiobjective in nature, it is often difficult to isolate a small region of good design space which can be accurately represented by a low-order polynomial response surface model [33]. Therefore, it is necessary to investigate alternative statistical methods that have sufficient flexibility to build accurate global approximations of the design space.

Kriging

Kriging evolved from the field of geostatistics [34] and has become popular in the area of spatial statistics [35]. The values of the predictor variables, from a spatial perspective, are points in the multi-dimensional predictor space. Some form of spatial correlation between points in the predictor space is assumed, and this correlation is used to predict response values between observed points.

The general kriging form is a combination of a polynomial model and departure of the form:

$$y(x) = f(x) + Z(x) \tag{2.2}$$

where y(x) is the unknown function of interest, f(x) is a known polynomial function of x, and Z(x) is the realization of a stochastic process with mean zero, variance σ^2, and non-zero covariance. The f(x) term is similar to the polynomial model in a response surface, providing a "global" model of the design space. Z(x) is a random process with mean zero and covariance which dictates the local deviations is as follows:

$$Cov[Z(x^i), Z(x^j)] = \sigma^2 R([R(x^i, x^j)]) \tag{2.3}$$

where R is the correlation matrix, σ^2 is the process variance and $R(x^i, x^j)$ is the correlation function between any two of the ns sampled data points x^i and x^j. R is a $n_s \times n_s$ symmetric, positive definite matrix with ones along the diagonal. The correlation function R is specified by the user.

Once a correlation function has been specified, predicted estimates, $\hat{y}(x)$, of the response, $y(x)$, at untried values of x are given by:

$$\hat{y} = \hat{\beta} + r^T(x) R^{-1}(y - f\hat{\beta}) \tag{2.4}$$

where y is the column vector of length ns (number of sample points) which contains the values of the response at each sample point, and f is a column vector of length ns which is filled with ones when f(x) in Eq. 2.2 is taken as a constant. In Eq. 2.4, $r^T(x)$ is the correlation vector of length ns between an untried x and the sampled data points $\{x^1, x^2, ..., x^{n_s}\}$ and is given by:

$$r^T(x) = [R(x, x^1), R(x, x^2), ..., R(x, x^{n_s})]^T \tag{2.5}$$

Finally, the $\hat{\beta}$ in Eq. 2.4 is estimated using the following expression.

$$\hat{\beta} = (f^T R^{-1} f)^{-1} f^T R^{-1} y \quad (2.6)$$

When f(x) is assumed to be a constant, then $\hat{\beta}$ is a scalar which simplifies the calculation of Eq. 2.6 and all others involving $\hat{\beta}$.

Kriging is extremely flexible due to the wide range of correlation functions $R(x^i, x^j)$ which can be chosen. Depending on the choice of correlation function, kriging can either "honor the data", providing an exact interpolation of the data, or "smooth the data", providing a non-exact interpolation [35]. In addition, kriging incorporates the spatial correlation of the data, while other classical statistical procedures do not. Another advantage of the kriging over other techniques is its ability to quantify the estimation variance which is important to define the precision of the resulting estimates [36]. Therefore, kriging does show the ability for creating surrogate model for complex systems.

Despite its advantages, kriging has several limitations. First, the usage of kriging metamodels in actual engineering design is still limited. One reason may be that the estimated parameters of a kriging model are computationally intensive to obtain, and the assumptions related to the correlation functions are difficult to verify [33]. Another reason may be that extraneous curvature might also exist in the prediction between observed values [37]. In addition, the application of kriging in engineering design should have an important assumption that the simulation data for creating kriging surrogate models is accurate without error. Because kriging is an interpolation technique, predictions are equivalent to the observed performances at observation points. In other words, kriging is very sensitive to outside noise. In engineering design, the data for creating model usually comes from a Design of Experiments of original simulation models. These simulation models may include the uncertainty and errors caused by model simplifications, especially for complex models. Therefore, the model from kriging may not always be accurate enough.

For complex systems design, the statistical methods should satisfy several requirements. First, they should be easy to use. The design tasks, system couplings and subsystem models have already introduced much complexity into the design process. It is unreasonable to introduce unnecessary additional complexity in statistical methods. Secondly, the statistical method should have the ability to fit both linear and nonlinear model accurately. Thirdly, the statistical method should be insensitive to the noise in the simulation data because the data for creating surrogate model comes from original subsystem models which may include uncertainties. A comparison between response surface method and kriging model in terms of requirements for statistical methods in complex systems is shown in Table 2. 2.

Table 2. 2 - A comparison between response surface model and kriging model in term of requirements for statistical methods in complex systems

Requirements for statistical methods in complex systems	**Response surface model**	**Kriging model**
Easy to use	Yes	No
Flexible to fit nonlinear models accurately	No	Yes
Insensitive to noise	Yes	No

Response surface models are widely used in current engineering design and a very easy to implement. The regression function of a response surface model is based on the whole data set, individual noise points do not influence the regression model very much, especially for lower order response surface models. However, this method has a serious limitation that it cannot model accurately nonlinear functions of arbitrary shape. High order response surfaces may include instabilities, and it may also be difficult to take a sufficient number of sample points in order to estimate all of the coefficients in the equation, especially when the computational cost of simulation data is high.

Kriging is more flexible than response surface modeling due to the freedom in the choice of correlation functions. This method can fit nonlinear data much better than response surface model. However, the mathematics of kriging is very complicated and much of the terminology and concepts are unique to geostatistics. Kriging has been criticized as difficult to implement [36]. In addition, because kriging is an interpolation method instead of a regression method, kriging may be seriously sensitive to noisy data. In engineering design, the purpose of the meta-modeling techniques is to replace computationally intensive original model based on the DOE data. However, the DOE data may not be accurate enough if uncertainty has already existed in original models.

Therefore, it is necessary to explore an alternative statistical method to satisfy all requirements of complex systems listed in Table 2. 2. Local regression is introduced in this thesis as promising statistical method for complex systems design.

Local Regression

Local regression was proposed by Cleveland [38] and further developed by Cleveland and Devlin [39]. The basic idea of the local regression is that a low-order polynomial is fit to a subset of the data with explanatory variable values near the point whose response is being estimated. Weighted least squares are used to fit the polynomial, giving more weight to points near the estimation points and less weight to those further away. The value of the regression function of the estimation point is obtained by evaluating the polynomial by using the explanatory variable values for the data point. Several important parameters of the local regression method should be considered in implementation, including the bandwidth, the degree of local polynomial, and weight function.

Mathematically, local regression is similar to a response surface model, since the least squares regression method is both applied to fit the polynomial. However, local regression is much more flexible than response surface model due to its regression in local domain. Strong ability to fit nonlinear data accurately is the biggest advantage of local regression. Moreover, good fitting in local domain does not mean sensitivity to noise in local regression. The robust version of local regression was introduced by Cleveland [38] to reduce the sensitivity to the noise. Although local regression is a computationally intensive method, which caused limited application in industry, it is no longer a problem in current computing environment, unless the data sets being used are very large. Since the Design of Experiments in engineering design is to avoid large expensive simulations, the computational cost of local regression method is not a problem in engineering design.

Therefore, local regression is an appropriate statistical method to use in complex systems design, because it can satisfy all following requirements: it is easy to use; flexible to fit nonlinear models; and insensitive to noise. The details of the mathematical concepts of local regression are discussed in Chapter 3.

Besides the accuracy of the meta-model, the efficiency of solution search is another limitation of current robust design for complex systems. In the next section, solution search methods are studied.

2.3 SOLUTION SEARCH METHODS

As discussed in Section 2.1, IDEM is a promising method to be modified to satisfy the requirements for complex systems design. However, the discrete function evaluation causes many limitations in its capabilities. It is necessary to replace the exhaustive search type of evaluations by continuous solution search methods. In Section 2.3, a discussion of some popular solution search methods in engineering design is presented. Section 2.3.1 begins with the introduction of Genetic Algorithms. Then, the Pattern Search is discussed in Section 2.3.2. Section 2.3.3 contains a detail explanation of the Adaptive Linear Programming Algorithm used in DSIDES, which is useful in solving nonlinear, multi-objective design problems. This section concludes with the comparisons of three methods.

2.3.1 Genetic Algorithm (GA)

The concept of Genetic algorithms was developed by Holland and his colleagues in the 1960s and 1970s [39]. Genetic algorithms (GAs) are efficient solution search methods based on Darwinian principle of survival of the fittest. In these methods, the mechanics of natural selection and genetics are simulated artificially so as to explore efficient solutions of a given problem. Genetic algorithms consist of three genetic operators: selection, crossover and mutation.

Genetic algorithms start from a population that is a randomly selected initial solution set. The search for a global optimal solution is conducted by moving from the initial population of individual variables to a new population using genetic operators, such as selection, crossover and mutation. Each individual is modeled as a fixed length string of symbols that is called a chromosome and it represents a candidate for the optimal solution. Starting with a randomly selected population, the GA operators perform crossover or mutation on the chromosome in order to produce new generations so that the solution is closer to the optimal one. The operation is based on the selective nature, in which the best candidates are chosen as parent based on the fitness so that new generation holds the best genetic heritage.

Fitness function is used to measure for the quality of an individual within the population, which assigns a fitness value to each individual. The basic GA optimization procedure is to process highly fit individuals in order to produce better individuals as the search progresses. Typically, a genetic algorithm contains four major steps, i.e. fitness evaluation, selection, recombination and creation of a new population. The simplified flow chart of a genetic algorithm is shown in Figure 2. 12.

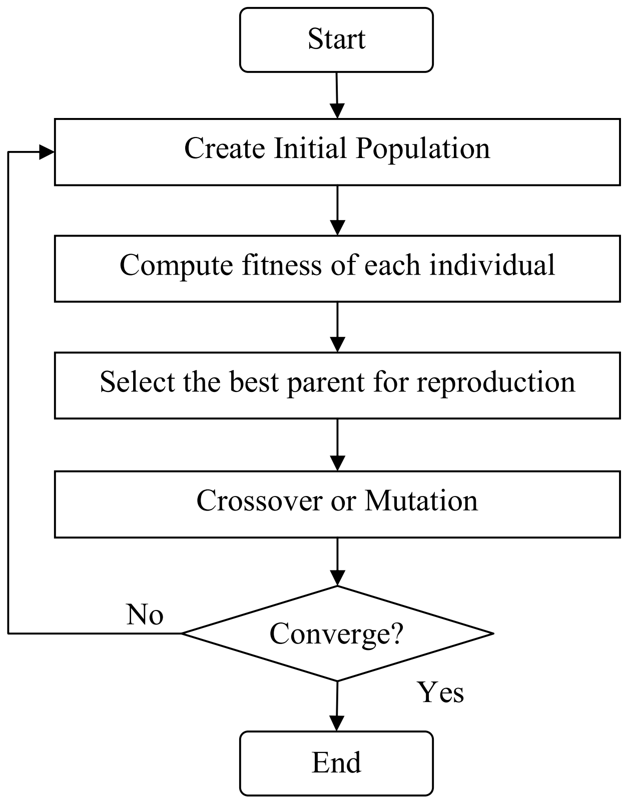


Figure 2. 12 - Flow chart of a genetic algorithm

The natural size and complexity of real-life problem models require approximations in order to accommodate the capacity of the solver. In these models, many of variable interactions are non-linear relationships, which traditional optimization approach may not provide viable alternatives, but genetic algorithms may be able to do. However, due to the advantages and disadvantages, genetic algorithms should not be considered as a replacement for other existing optimization approaches, but as another alternative which the designers can use [40].

Genetic algorithms have a number of advantages. First, they can be applied in any problem where optimization is needed. Secondly, GAs can use parallel computing due to the multiple offspring which thus makes GAs ideal for large problems, where evaluation of all possible solutions in serial would be difficult if not impossible. Thirdly, the designers who apply GAs do not need to worry about the starting points for the optimization, which may seriously affect the end solution negatively in the traditional approaches. In GAs, the initial population is randomly selected and bad products are simply discarded in the process. Moreover, the GAs are easy to implement and fit themselves well into other approaches or design process.

The greatest advantage of the genetics algorithms, that is they find a solution through evolution, is also the biggest disadvantage [41]. Evolution is inductive, that is, life does not evolve towards a good solution, but it evolves to eliminate bad ones and keeps away from bad circumstance. Therefore, usually GAs take more time to converge than traditional approaches. Thus, the computational cost may be higher for small problems. The nature of evolution also causes the second disadvantage. GAs usually cannot guarantee that they reach a global optimal solution, because they do not directly explore the optimal solution. However, they still always find the best local optimal solution, which may be closed to the optimal one. Furthermore, the accuracy of the solution GAs find depends on the fitness function or fitness value. Although GAs do not require any knowledge of how to get a solution for the problem to be solved, they do require exact information of the fitness function or value in order to achieve a high fitness. Unfortunately, in some complex problems with complicated constraints, it may be difficult for the fitness functions to manage and quantify possible infeasibility.

2.3.2 Direct Search Methods

Direct search is a method for solving optimization problems without requiring any gradient information of the objective function. Instead of using information about the gradient or higher derivatives to search for an optimal point as more traditional optimization methods do, a direct search method searches a set of points around the current point, searching one where the value of the objective function is lower than the value at the current point [42].

Although there are more sophisticated numerical techniques, such as the globalized quasi-Newton method, direct search methods are still popular in practice due to several good reasons. First, direct search methods work well in solving problems for which the objective function is not differentiable, or is not even continuous [42]. Second, the globalized quasi-Newton method may not be applicable to many nonlinear optimization problems. In such cases, direct search methods are an alternative. Features unique to direct search methods often avoid the problems that may plague more sophisticated methods [43]. Third, direct search methods are straightforward and simple. The requirements from a user are minimal and usually only settings of few parameters are required. Due to this feature, direct search methods are usually employed as preliminary solution search for some complex optimization problem. The direct search calculation can be used as a “hot-start” for one of sophisticated techniques, which can achieve global optimal solutions quickly.

The popular direct search methods can be classified into three categories, pattern search methods, simplex methods (not the simplex method for linear programming), and methods with adaptive sets of search directions [43]. In this thesis, pattern search methods are implemented as the solution search method to find design specifications. The pattern search method used in this thesis is in Genetic Algorithm and Direct Search

ToolboxTM 2 of the Matlab. The introduction of pattern search is leveraged from the Toolbox User's Guide [42].

Pattern search methods are characterized by a series of exploratory moves that evaluate the behavior of the objective function at a pattern of points, called a mesh, around the current point which is computed at the previous step of the algorithm. The algorithm forms the mesh by adding the current point to a scalar multiple of a fixed set of vectors, which is called a pattern. If the algorithm finds a point in the mesh that improves the objective function at the current point, the new point becomes the current point at the point at the next step of the algorithm, which is called successful poll. If the algorithm fails to find a point in the mesh that improves the objective function, the current point stays the same at the next iteration, which is called unsuccessful poll. After each poll, the algorithm changes the value of the mesh size. The default is to multiply the mesh size by 2 after a successful poll and by 0.5 after an unsuccessful poll. The algorithm stops when the mesh size reaches the minimum defined by users.

Patter search is easy to use, but it also has several limitations. First, it may get stuck in local minimum and different starting points analysis may be necessary. This situation usually happens when model is nonlinear or constraints are complicated. Secondly, pattern search may be costly, especially when the starting point is far away the optimal point. However, pattern search is still more efficient than Genetic Algorithm and requires fewer function calls.

In summary, pattern search is an efficient solution search method when there are not many complicated constraints. It is usually used as a preliminary solution search tool to find minimal solution with known global convergence properties and the solution is used as a reference for more sophisticated techniques.

2.3.3 Adaptive Linear Programming (ALP) Algorithm

Adaptive linear programming (ALP) algorithm is considered as the highest potential for being used to solve a range of Decision Support Problems in engineering design. There are three important features contributing to the success of the ALP algorithm, namely, [18]

- The use of second-order terms in linearization
- The normalization of the constraints and goals and their transformation into generally well-behaved convex functions in the region of interest
- An "intelligent" constraint suppression and accumulation scheme

Mathematically, the ALP algorithm is a modified second-order algorithm, which needs the derivatives of the constraints and goals as well as the values of these quantities. The derivatives are determined numerically by the central difference formula.

A block diagram of the implementation of the ALP algorithm is shown in Figure 2. 13. The user should prepare the input data file for the software implementation of the algorithm in the form of a DSP template. The data file includes the information such as the problem size, the names of the variables and constraints, the bounds on the variables, the linear constraints, and the convergence criteria. The FORTRAN or Java routines are used to evaluate the nonlinear constraints and goals, to input data required for the constraint evaluation routines and the design analysis routines, and to output results in a format set by users. There are two cycles in the whole algorithm, that is, analysis cycle and the synthesis cycle. In the design of single problem in a complex system, it is desirable to use the design-analysis interface associated with the analysis cycles, while it has been found necessary to use both of the interfaces for solving large, analysis-intensive and complex problems, such as the multiscale design problems. Once the nonlinear compromise DSP is formulated, it is approximated by linearization. At each stage, the solution of the linear programming problem is obtained by a Multiplex algorithm [44]. The deviation function that is given in the mathematical form of the template can be implemented in two ways:

1. In the Preemptive form as a lexicographic minimum of the goal deviation variables.
2. In an Archimedean form as a weighted function of the goal deviation variables.

The details of the ALP can be found in [18].

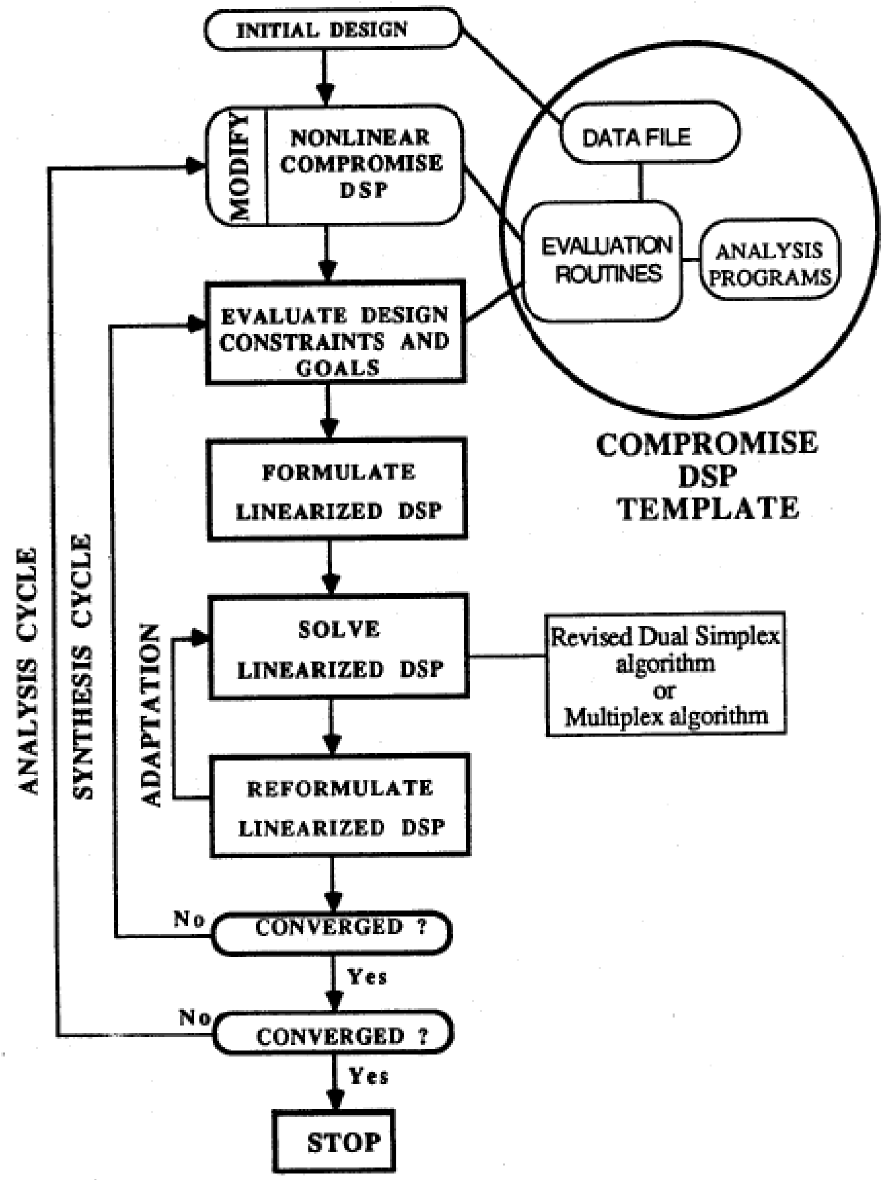


Figure 2. 13 - Implementation of the ALP algorithm for solving compromise DSPs [18]

ALP is developed to solve compromise DSPs based on the goal programming and mathematical programming techniques. This algorithm can solve an approximation of the problem exactly, which is just what compromise DSPs require. The ALP algorithm has been implemented in DSIDES. DSIDES embodies the principles espoused in the decision support problem technique. The decision support problem technique and DSIDES have been successfully used in the conceptual design of ships and airplanes and in the design of aircraft tires, damage-tolerant structural and mechanical system, and composite materials. [18] The DSIDES system is particularly appropriate for solving multi-criteria problems involving Boolean and continuous variables, that is, the problems that include both selection and compromise.

Although ALP algorithm is very efficient in solving compromise DSPs, there are some disadvantages that limit its applications. First, the ALP algorithm is only capable of handling Boolean and continuous variables. If there are discrete or integer variables, it is difficult if not impossible to implement the ALP algorithm to solve the design problems. Secondly, some of the linearized constraints in the ALP algorithm may render the feasible design space infeasible if the system constraints are highly nonlinear. In this case, ALP algorithm temporarily or permanently suppresses these constraints and restores them in the subsequent synthesis cycles. Either these permanently suppressed constraints are redundant for the particular case or there is an error in their formulation. In either case, it is left to designers to analyze the situation and take the necessary corrective action if possible. Thirdly, in order to implement the ALP algorithm, designers are required to prepare a data file and have all information about the design problems, especially the detailed constraints information. However, sometimes the designers do not have sufficient information about the constraints, especially in original design, in which not much existing mathematic functions are available. In such case, the ALP algorithm may not be an appropriate choice to solve the problem.

2.3.4 Comparisons of Different Solution Search Algorithms

The comparisons of three algorithms are shown in the following table.

Table 2. 3 - The comparisons of three different algorithms

Algorithm/ Characteristics	**Genetic Algorithm**	**Direct Search Methods (Pattern Search)**	**Adaptive Linear Programming**
Computational Cost	High, especially for small problems	Relatively high	Normal
Accuracy of solution	Close to optimal solution	Usually, optimal solution	Optimal solution under linearized constraints.
Case with local minima	Not influenced	Need different initial estimations	Need different initial estimations
When to use?	Complex or original design without much knowledge about how to get a solution	Most parametric design problems	Compromise DSPs with detailed constraint functions

Three algorithms are appropriate for different design problems. For instance, if the designers are working with complex or original design without sufficient knowledge how to get the solution, genetic algorithm may be the best one to solve the problem. Moreover, the genetic algorithm is also easy to solve the design problems with discrete and integer variables. Although the computational cost is sacrificed, it is helpful for the designers to find the preliminary solutions and gain more information about the design problem. Direct Search Methods are more efficient to solve problems with most parametric design problems with only a few local minima. However, in order to make sure the solution is the global optimal solution, the designers have to restart the optimization with different initial estimations. These methods can be employed as the preliminary solution exploration and the solutions can be used as starting points for more sophisticated techniques. Adaptive linear programming is very useful to solve the compromise DSPs with detailed constraint functions. With DSIDES, it is also easy to implement. However, it requires more design information than directed grid search and it has the same limitations as DGS when the problems have many local minima or some variables are discrete.

Therefore, none of these algorithms is the best. Designers have to make decisions to choose the appropriate method to solve a specific design problem. All of these methods are possible methods to replace the exhaustive search type of evaluation process in the IDEM. In this thesis, grid search is used as solution search method.

2.4 RESEARCH GAPS IN ADAPTIVE DESIGN SYSTEMS

The primary purpose of the literature review in Section 2.1 – Section 2.3 is to identify knowledge gaps relating to the key concepts of this thesis, a more efficient and accurate robust design approach for systems design. The knowledge gaps identified in this thesis are intended to improve the efficiency and accuracy of the robust design method for complex systems.

2.4.1 Research Gap Relating to the Efficiency of Inductive Design Exploration

In Section 2.1, the existing robust design method, the Inductive Design Exploration Method, is considered as a promising method to be employed in complex systems design. However, the limitation of the IDEM in computation efficiency constrains its capability in complex systems problem with a large number of design variables. This limitation arises from the Discrete Function Exploration procedure in the IDEM and this procedure may not be necessary or useful for the design problems other than materials design. The purpose of this discrete exploration is to provide designers with sufficient design freedom in each step as much as possible. Although the parallel computing techniques can be employed to reduce the computational cost, it increases the complexity of the design process as well. Since most engineering design processes are based on an efficient optimization routine, discussed in Section 2.3, thereby, **is it possible to replace the discrete exploration process by efficient solution search method?** This is the primary research question in this thesis, as introduced in Section 1.3.2.

This research gap may be filled up by modifying the assumption of the IDEM. The large design freedom is necessary due to the challenges of material design. For instance, major sources of uncertainty in processing, microstructure, model, etc., must be taken into consideration, since they can dominate the configuration of the design process. In addition, process capabilities may constrain specific microstructure obtained from the design process, and thermodynamics and kinetics considerations may also limit microstructure solutions. Therefore, it is necessary for designers to obtain a large range of accessible solutions so that they have freedom to make decisions according to these constraints. However, this assumption may not be appropriate for adaptive design systems, in which sufficient information is available so that large design freedom is not necessary for designers to make decisions. In this thesis, the basic idea of dealing with uncertainty propagation in IDEM is accepted. A ranged set of robust solutions against the propagated uncertainty in the complex systems can be found by passing down the feasible solution range in an inverse manner. However, the ranged set is not assumed as large as possible in each step. In other words, the assumption that design freedom should be kept as large as possible for each step is not accepted in this thesis. By modifying this assumption, it is possible to implement solution search method to find the best ranged set of design solution and the size of the range can be defined by designers instead of discrete exploration.

2.4.2 Research Gap Relating to the Accurate Fit of Nonlinear Subsystem Models

In Section 2.1, all types of robust design approaches are studied. Meta-modeling techniques are widely used to reduce computational cost. The response surface is the most popular approach as the statistical method. However, this method has limitations in fitting nonlinear models. Kriging was also recommended to replace response surface method in the design process [45], but it is an interpolation technique rather than a regression method so that it may be very sensitive to the noisy data. The type III robust design, the RCEM-EMI and robust design method for model chain, the IDEM, takes uncertainty bounds of models into account to deal with model uncertainty. Since the uncertainty bounds of models are usually the confidence intervals of the response surface model, the model may be still inaccurate when fitting highly nonlinear models, which is also recognized in [4]. Therefore, it is necessary to find an alternative statistical method to avoid these limitations. **How to improve the accuracy of the surrogate model fitting nonlinear model?** This is the secondary research question to be answered in this thesis, as introduced in Section 1.3.2.

In section 2.4, different meta-modeling techniques, including response surface model, kriging model and local regression model are studied. After comparing the limitations of the response surface model and kriging model with the advantage of local regression model, it is recognized that the local regression model is an appropriate method to be introduced in the design process with the advantages including ease to use, good flexibility to fit nonlinear models and insensitivity to noisy data.

The validation square roadmap is illustrated in Figure 2. 14.

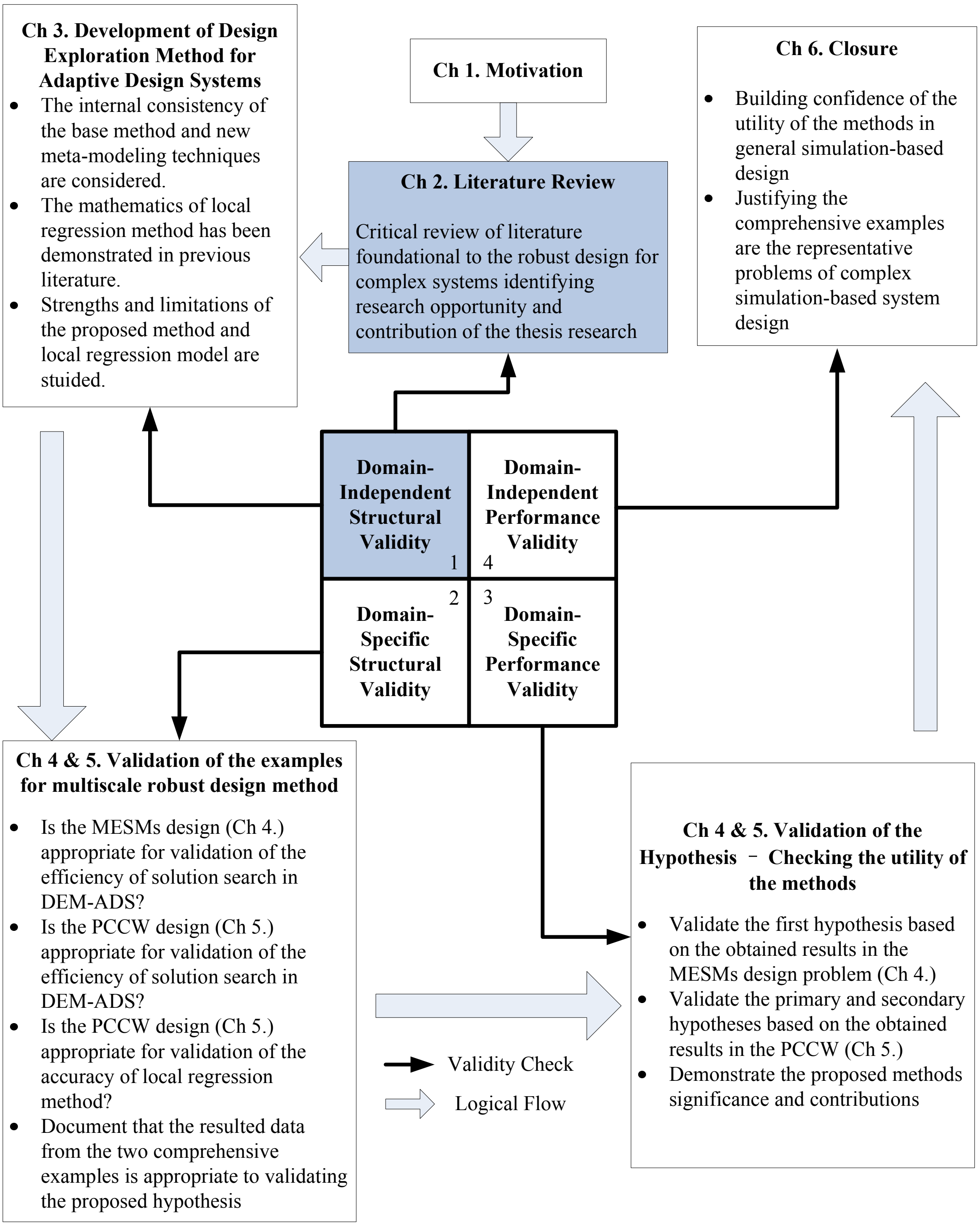


Figure 2. 14 - Validation Square roadmap

2.5 SYNOPSIS OF CHAPTER 2

Chapter 2 contains a review of robust design, meta-modeling techniques and solution search methods. The key research gaps identified in Chapter 2 are: the efficiency of the solution search process in the adaptive design systems and the accuracy of surrogate models. Based on the literature review, research opportunities are identified. The IDEM is effective in uncertainty management in system design, and it is possible to implement efficient solution algorithms to replace the discrete exploration process in the adaptive design systems so that the efficiency of solution search can be improved. In addition, it is shown that local regression model has the ability to flexibly fit nonlinear models and create surrogate models accurately. It is possible to implement the research opportunities identified in Chapter 2 to modify IDEM and introduce local regression model to address the research questions introduced in Chapter 1.

In next chapter, the research opportunities identified in Chapter 2 are implemented into the proposed methods to address the research questions. IDEM is modified to an inverse design exploration process in the design exploration method for adaptive design systems, which is proposed to improve the efficiency of solution search by efficient solution search algorithms. Local regression method is introduced into the design process to improve the accuracy of the surrogate model. Therefore, Chapter 3 provides the theoretical foundation for answering research questions, and Domain-independent Structural Validity can be completed in the next chapter.

CHAPTER 3
THEORETICAL FOUNDATIONS FOR THE DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS

The information presented in Chapter 3 provides the theoretical foundation for the remainder of this thesis. In this chapter, the generic formulation of a robust design for complex systems is presented. Formulation of the design exploration method for adaptive design systems is based on a previously developed multiscale robust design method, the Inductive Design Exploration Method [4], introduced in Chapter 2. It is formulated in response to Research Question 1: '*How can we control the propagation of uncertainty in the complex adaptive design systems efficiently?'* and Research Question 2: '*How can the accuracy of surrogate models for computationally intensive and nonlinear simulation models be improved?*' As suggested by the discussion in Chapter 2, IDEM is too computationally intensive to implement in general system design, and the response surface model widely used in engineering design is not an appropriate method to fit a nonlinear model, which is common in systems design. However, a modified design approach based on the IDEM and local regression model can address these problems.

Chapter 3 begins with an introduction of the overview of the design exploration method for adaptive design systems. The steps of the method and assumptions are introduced briefly. Then, system design clarification and design of experiments steps are described. Next, the step for regression methods is described and an alternative regression method, the local regression method, is introduced to fit nonlinear models. Then, the inverse design exploration process, which is the core of the proposed method, is discussed in details. Finally, the verification and validation of the propose method is presented by examining its domain-independent structural validity. Figure 3. 1 illustrates how Chapter 3 is connected to other ideas in this thesis.

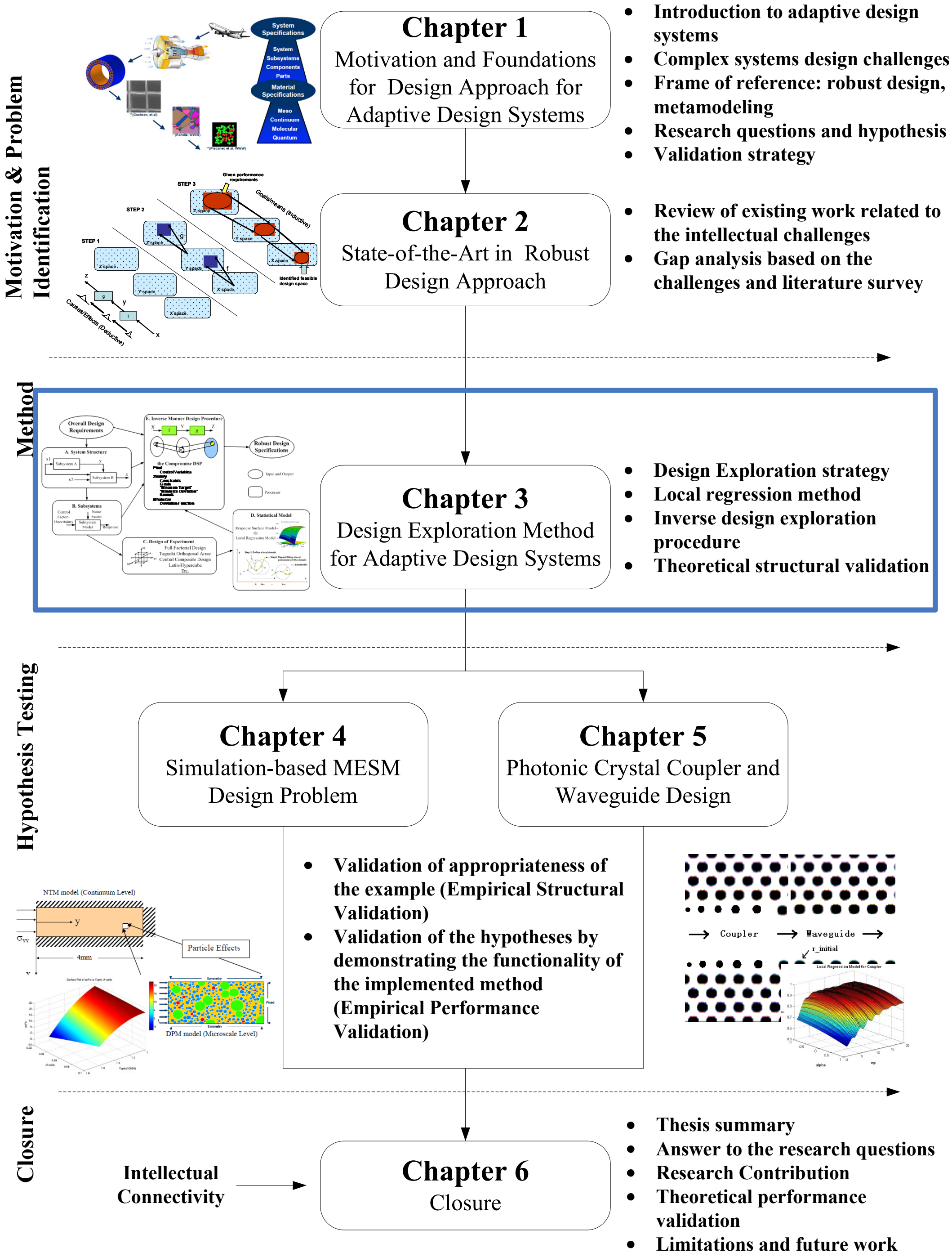


Figure 3. 1 - Thesis roadmap

3.1 AN OVERVIEW OF THE DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS

The main focus in this thesis is to develop the design exploration method for adaptive design systems (DEM-ADS) to find solutions against the uncertainty in systems design efficiently (Primary Research Question, Section 1.3). In order to address this challenge, it is decided that the potential method can be based on an existing method for facilitating robust solutions to systems design problems. The Inductive Design Exploration Method (IDEM) is selected as the base method for this thesis and modifications improve the efficiency of its solution search process. In addition, inaccurate simulation models provide another source of uncertainty in systems design. Therefore, local regression is introduced to improve the accuracy of the surrogate models (Secondary Research Question, Section 1.3).

3.1.1 Procedure of the Design Exploration Method for Adaptive Design Systems

The goal of the design exploration method for adaptive design systems is to reduce the uncertainty influence in systems design with more efficient solution search method than the original IDEM. The basic of the idea of the IDEM to manage uncertainty is inherited in this proposed method. The robust solutions against the uncertainty are ranged set of solutions found by passing the feasible solution range in an inverse manner, from desired given final performance ranges to the space of input variables. Therefore, the core of the proposed method is the inverse manner solution exploration, in which main modifications are made to adapt the IDEM to more general systems design problems. Figure 3. 2 illustrates the design exploration method for adaptive design systems steps. Simply speaking, there are five major steps involved, namely, “define system structure”, “classify design parameters and uncertainties for each subsystem”, “design of experiments”, “model regression” and “the inductive design exploration”.

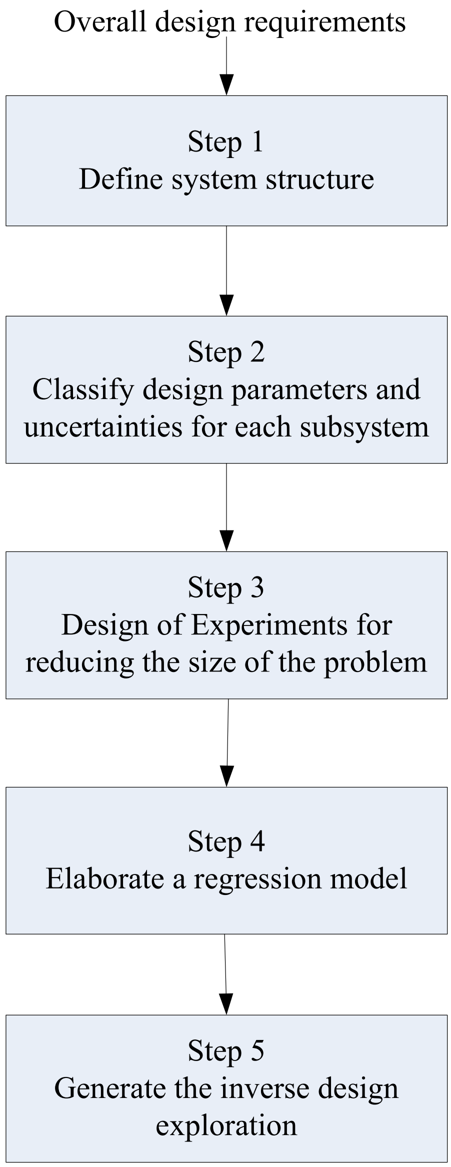


Figure 3. 2 - Steps of the design exploration method for adaptive design systems

In Step 1, the design problem should be carefully studied to determine the system configuration, including the inputs and outputs of the system, the number of subsystems and the couplings between subsystems and multi-level couplings. The necessary information in this step comes from the design task clarifications. In this step, designers can manage the complexity of the system by combining the subsystems, modifying the structures or splitting one complex subsystem into several simple ones, if necessary.

In Step 2, each subsystem should be studied. The purpose of this step is to classify all design parameters following the design principles used in robust design and to define the design space. In this step, the design parameter classification is the same as the first step in RCEM [16]. Different design parameters are classified either as control factors, noise factors, or response. Uncertainty is also considered associated with unstable operating environment, manufacturing processes or other factors. In this step, the design bound of each input variables and desired responses should be identified, which is important for defining design space and desired response space for the inverse manner design exploration step.

In Step 3, Design of Experiments (DOE) is to prepare simulation data for creating surrogate models and provide the information for further secondary experiments. The results of DOE can be used to identify the significance of main effects and omit trivial factors. In this step, the design space can be reduced in terms of the sampling results, and trivial input variables can be eliminated in order to reduce the complexity of the design problem. Designers can choose any one of the DOE techniques discussed in Section 2.2 in this step.

In Step 4, a statistical regression model is employed to fit the data from step 3. The purpose of this step is to replace the original expensive analysis programs with a fast analysis module. The results of the regression model can also increase the knowledge about the significance of different design variables, the interactions and uncertainties. In this paper, the response surface model and the local regression model are recommended as the statistical models to create surrogate models. The response surface model is very easy to use and it works well if models are not highly nonlinear. In the cases where models have nonlinear features, it is better to choose the local regression model which has better ability to fit nonlinear model accurately. The details of the local regression are discussed in Section 3.2.

In Step 5, the inverse manner design exploration process is employed to find ranged sets of solutions against uncertainty propagation in the model chain, which is derived from the original IDEM process. The details of the inductive design exploration process are introduced in Section 3.3.

The computing infrastructure of the design exploration method for adaptive design systems is illustrated in Figure 3. 3. The Step 1 is to clarify the design system and subsystems based on the design clarification and requirements. In Step 2, the design variables and uncertainty factors are studied for each subsystem. Design of Experiment is employed in Step 3 and the local regression model is implemented in Step 4 to create surrogate models of each subsystem which are more computationally efficient than original model with high computational cost. In Step 5, the inverse design exploration is employed to find a ranged set of solutions against uncertainty propagation in the model chain.

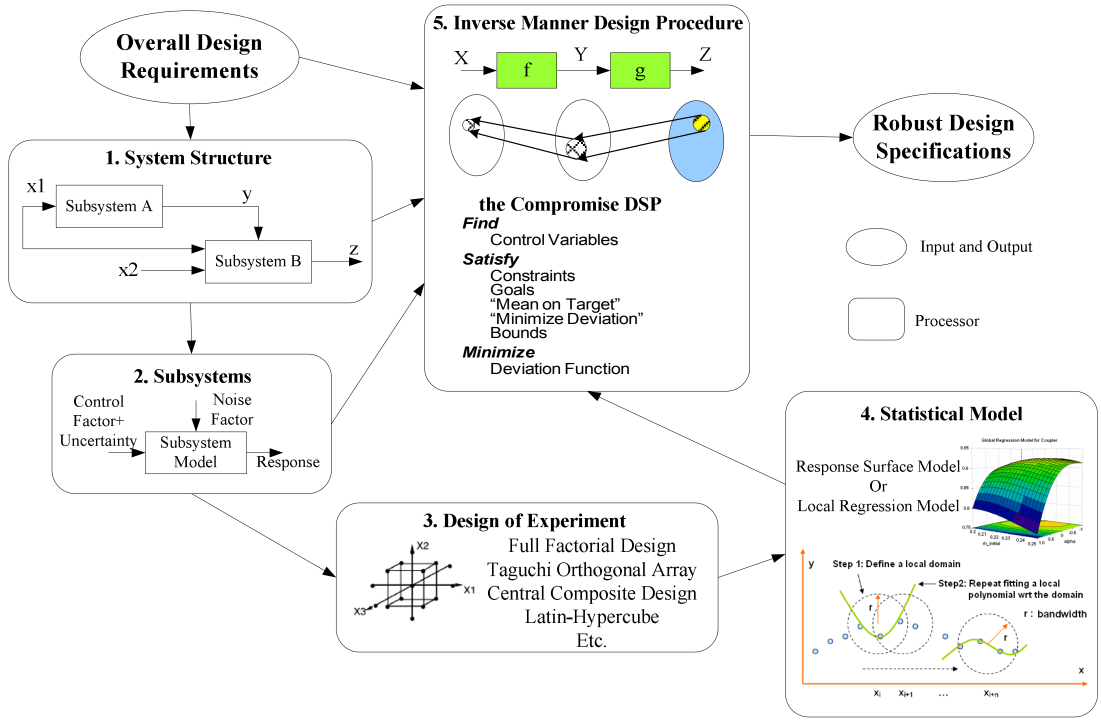


Figure 3. 3 - Computing infrastructure of the design exploration method

3.1.2 Assumption of the Design Exploration Method for Adaptive Design Systems

There are several important assumptions in the design exploration method for adaptive design systems. One assumption in this method is that the desired response space should be achievable. The solution search process of the proposed method is a top-down solution search procedure, and the solution is obtained from the desired response range. Therefore, the desired response range should exist, which means that design requirements and objectives should be reasonable and achievable. This assumption is the foundation for the proposed method. In IDEM, which is developed for multiscale material design, the mapping relationship between the input and output is unknown, and designers have little information about the possible performance of the tailored materials. Therefore, the discrete exploration process is necessary in the IDEM to explore the whole design space and check if the desired objectives are achievable. This assumption can be satisfied in the adaptive design systems problem. As introduced in Section 1.1, in the adaptive design, designers implement existing technology and solution principles to different design objectives and constraints. Therefore, in this kind of design problem, designers have already known much about the subsystems, so that it is possible that they are able to identify achievable desired objectives.

Another assumption is that designers do not need unnecessarily large design freedom. In the IDEM, designers explore the whole design domain and filter all feasible design solutions for each step and keep the design freedom as large as possible in each design step. For multiscale materials design, large design freedom is necessary because the design problems themselves also have many uncertainties. The design problem may also be modified in later stages in order to satisfy other materials development constraints, such as stiffness, heat tolerance, etc. In addition, the designers also have to deal with uncertainty propagation in the model chain. In the adaptive design, designers have already obtained sufficient information and knowledge about the subsystems, the design problems can be defined more clearly. It is not necessary to spend huge computational cost on achieving large design freedom. Instead of finding all of feasible solutions, designers define the size of the feasible solution range in consideration of uncertainty analysis and possible slight modifications of the design problems in detail design stage, and then find the most appropriate solution range. Therefore, the solutions of the design exploration method for adaptive design systems must be a subset of the IDEM.

The third assumption of this method is that the solution range closer to the middle of design space is better. This assumption is the same as the IDEM. The solution is considered more likely to be satisfactory if the mean of the solution moves farther from the constraint and system requirement boundary. Solutions that are far from the boundaries of the feasible design space will remain within the feasible design space in the presence of slight variation, meaning that these solutions are insensitive to, or robust to variation. Because of this assumption, the solution evaluation metrics, the Error Margin

Index (EMI), is also inherited in the proposed method. The assumption comparisons of the IDEM and the proposed method are shown in Table 3. 1 as the summary.

Table 3. 1 - Assumption comparisons of the IDEM and Design Exploration Method for Adaptive Design Systems

The Inductive Design Exploration Method	**The Design Exploration Method for Adaptive Design Systems**
The input and output mapping relationship is uncertain, so that it is necessary to discretely explore the whole design space to find out if the desired response is achievable.	Designers have sufficient information about the design problem so that the design objectives (desired responses) are achievable in adaptive design systems.
Large design freedom is necessary and the design freedom should be maximized in each steps in order to find feasible solutions.	Large design freedom is not necessary for the design problems with sufficient information. Designers just need to keep design freedom large enough for uncertainty or possible design parameter modifications.
Solution range closer to the middle of design space is better.	

3.2 CLARIFICATION OF DESIGN SYSTEM

In this section, a process for clarifying the design system, which is Step 1 and Step 2 of the construct of the design exploration method for adaptive design systems is discussed. This task is an important step since the design goals, design parameters, uncertainty identification and system structure are determined in this process.

In Step 1, system couplings and design goals need to be identified from the system modeling and system design requirements. In this step, designers should identify parameters indicating the system capacity for a specific purpose when designing a system and model couplings. Depending on the type of goals identified, the design preference can be classified as “smaller is better”, “nominal is better” or “larger is better”. For each type of goals, an upper requirement limit, upper and lower requirement limit, and a lower requirement limit can be identified.

Once the system couplings and design goals are identified, the next step is to identify the control and noise factors in each subsystem model that affect the system performance. Factors can be easily controlled by designers are design variables while those that cannot be controlled are noise factors. The number of control and noise factors determines the number of simulations that necessary for establishing meta-models in Step 3 and Step 4.

After design factors are identified, it is also important to identify uncertainty in each model. As discussed in Section 2.1, uncertainty in a subsystem model can be variability in control and noise factors, variability embedded in model behavior, assumption and idealization of analysis model or experiment, and limitation of data acquisition. Uncertainty identification is an important task in the design exploration method for adaptive design systems.

3.3 DESIGN OF EXPERIMENTS (DOE) AND MODEL REGRESSION

Based on the control and noise factors identified in the previous section, it is necessary to design experiments to reduce the computational cost of complex models. As discussed in Section 2.3, there are many DOE techniques available for characterizing a model response in terms of the control and noise factors. In the design exploration method for adaptive design systems, different DOE techniques can be implemented for different design problems.

Different meta-modeling methods can be used to fit the DOE data. In the RCEM, response surface modeling is used to create the regression method. As discussed in Section 2.3, response surface modeling is useful for many engineering design problems. However, for some models with highly nonlinear DOE data, the response surface modeling may not fit the data well unless very high order polynomials are used. In this thesis, an alternative regression method, the local regression method, is introduced to fit the highly nonlinear model easily. This method is proposed to create the more accurate regression model with lower order polynomials than response surface modeling. In this section, the local regression method is introduced in detail.

3.3.1 Background of Local Regression Method

It is a common approach to approximate the system response by using relatively inexpensive meta-models in the complex system design. Sometimes, the traditional regression methods do not perform well or cannot be effectively applied without undue labor. Currently, many multidisciplinary systems usually contain complex subsystems, such as highly nonlinear design of experiment results and design requirements. Sometimes, there is only observation or experiment result existing. Local weighted scatter plot smoothing (LOESS) is one of many "modern" modeling methods designed to address these situations. Local regression combines the characteristics both of linear least squares regression and nonlinear regression. The most attractive feature of this method is that designers are not required to specify a global function of any form to fit a model to the data, only to fit segments of the data [46]. This feature makes LOESS appropriate to be employed in the original modeling tasks where no existing nonlinear functions are available to fit a highly nonlinear model, which is common in the material design problems. In addition, in comparison to classical fitting global parametric functions, local regression substantially increases the domain of the surface to be estimated without distortion. Although the trade-off for these features is increased computational cost, this method is consciously designed to take full advantage of current computational ability to achieve the goals that are not easily achieved by traditional approaches.

LOESS is originally proposed by Cleveland [38] and further developed by Cleveland and Devlin [39]. It is more descriptively known as locally weighted polynomial regression. The basic idea of the local regression is that a low-degree polynomial is fit to a subset of data with explanatory values near the point whose response is being estimated. The explanatory values are the points in each local domain, which is introduced in Section 3.3.2. The weighted least squares are used to fit the polynomial, giving more weight to points near the estimation points and less weight to those further away. The value of the regression function of the estimation point is obtained by evaluating the polynomial by using the explanatory values for the data point. The local regression process is completed when regression function values have been computed for all selected points in the data set. The process of local fitting is illustrated in Figure 3. 4.

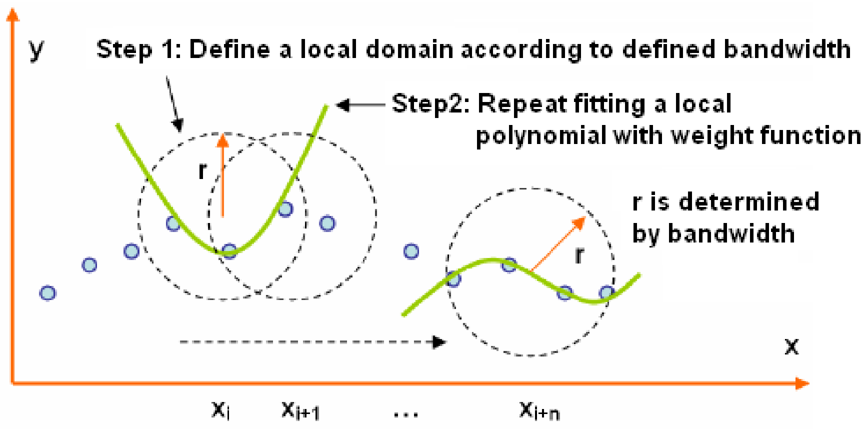


Figure 3. 4 - Local fitting with specific bandwidth and local polynomials (modified from [47])

3.3.2 Important Components of Local Regression Method

Several important parameters of the local regression method should be considered in implementation, including the bandwidth, the degree of local polynomial, and weight function.

A. Bandwidth

The bandwidth or smoothing parameter is a user-specified input to the procedure to determine how much of the data is used to fit each local polynomial. This parameter has a critical effect on the local regression result.

If the bandwidth is too small, insufficient data falls within the smoothing window, and a noisy fit or large variance fit will result. On the other hand, if the bandwidth is too large, the local polynomial may not fit the data well within in the smoothing window, and the most important and attractive features of the local regression may be completely lost.

The simplest way to specify the bandwidth is to make it constant for all data points. However, samples from experimental design, such as Latin-Hypercube, have data with a non-uniform distribution, which can obviously lead to problems with empty neighborhoods. Therefore, instead of using a constant bandwidth, a nearest neighbor bandwidth is usually adopted, so that the local neighborhood always contains a specified number of points. For a smoothing parameter α between 0 and 1 and the total number of the points, n, there are always k points in the bandwidth, in which $k = n \cdot \alpha$. Since the total number of the points is constant, it is the smoothing parameter α that determines the bandwidth. The value of α is usually determined by GCV score and plot, which is discussed in Section 3.3.4.

The local quadratic fits for a nonlinear data set using four different values of bandwidth, α is shown in Figure 3. 5. The smallest bandwidth α =0.2 produces a much noisier fit than the largest bandwidth α=0.8. α=0.8 has make the fit over-smoothed, because it does not track the data well. It depends on the designers and analysts to choose which bandwidth to be used from α=0.4 and α=0.6. Therefore, the local regression model is quite flexible. It can either "honor the data" or "honor the trend". By using an appropriate bandwidth value, the local regression model can well fit the nonlinear data even with noise, which is better than kriging method, as discussed in Section 2.2.

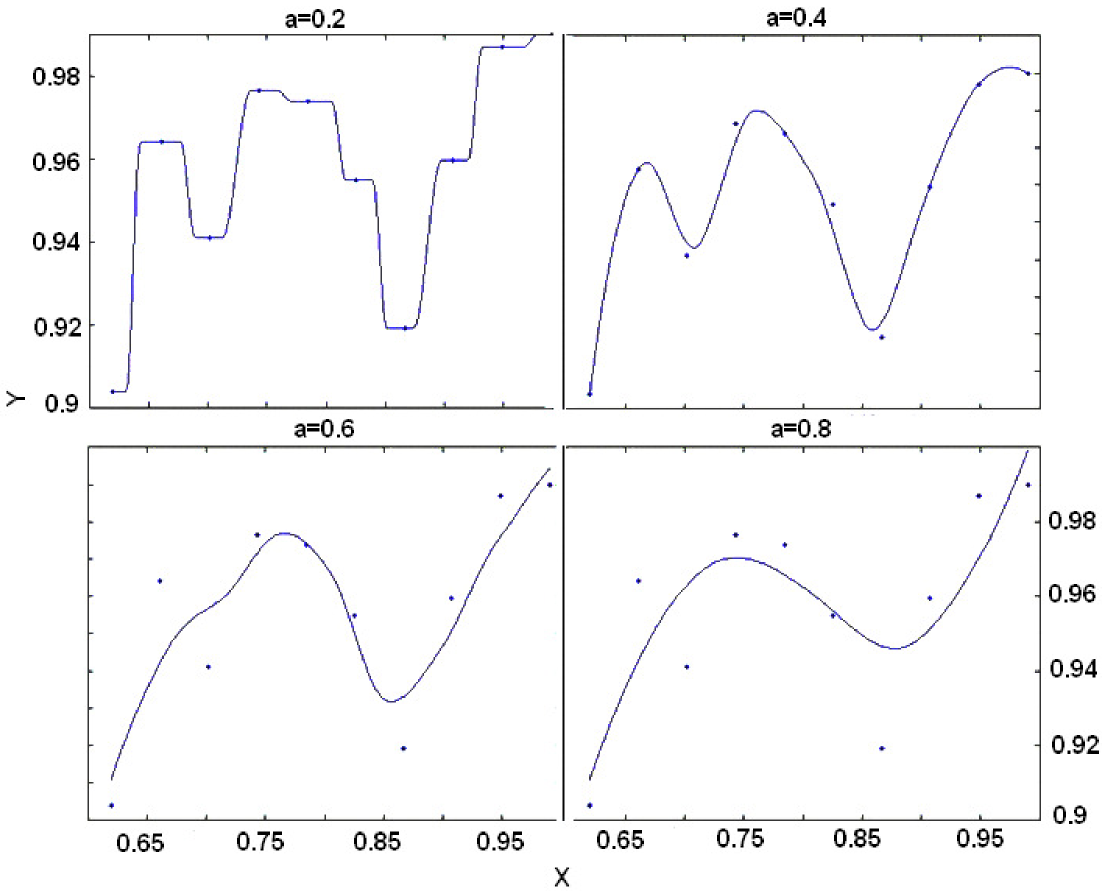


Figure 3. 5 - Local fitting at different bandwidths (α =0.8, 0.6, 0.4 and 0.2)

B. Local Polynomial Degree

The degree of the local polynomial affects the bias-variance trade-off. For local regression, the degree is set as first or second order; that is, either locally linear or locally quadratic. A high polynomial degree can always provide a better approximation to the underlying mean than a low one, but it also yield models which are not really in the spirit of local regression. Local regression is based on the idea that any highly nonlinear data can always be approximated well in a small neighborhood by a low order polynomial.

It often suffices to choose a low degree polynomial and to choose the bandwidth in order to obtain a satisfactory fit. Thus, the common choices are local linear and local quadratic polynomials.

C. The Weight Function

The weight function also affects the visual quality of the fitted regression curve although it has less effect on the bias-variance trade-off than the local polynomial degree. The weight function gives the most weight to the data points nearest the point of estimation and the least weight to the points that are far away. The implementation of the weights is based on the idea that points near each other in the explanatory variable space are more likely to be related to each other than points that are further apart.

The traditional weight function used for local regression is the tri-cube weight function [48]:

$$w(x) = \begin{cases} (1-|x|^3)^3 & for\,|x| < 1 \\ 0 & for\,|x| \geq 1 \end{cases} \tag{3.1}$$

3.3.3 A Mathematical Example

If h is the bandwidth, for $x-h \le x_i \le x+h$, a local quadratic approximation is [48]

$$\mu(x_i) \approx a_0 + a_1(x_i - x) + \frac{a_2}{2}(x_i - x)^2 \tag{3.2}$$

A general polynomial of degree p would look like this [48]:

$$u(x, x_i) = \sum_{k=0}^{p} a_k \frac{(x_k - x)^k}{k!} \tag{3.3}$$

In the above equation a_i is an unknown coefficient and requires to be solved in order to interpolate the local regression value at x. The following formula should be used [48]:

$$\begin{bmatrix} a_0 \\ \vdots \\ a_p \end{bmatrix} = (X^T W X)^{-1} X^T W Y \tag{3.4}$$

$$X = \begin{bmatrix} 1 & \cdots & \dfrac{(x_0 - x)^n}{n!} \\ \vdots & \ddots & \vdots \\ 1 & \cdots & \dfrac{(x_n - x)^n}{n!} \end{bmatrix} \tag{3.5}$$

$$W = \begin{bmatrix} w(\frac{x_0 - x}{h}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & w(\frac{x_n - x}{h}) \end{bmatrix} \tag{3.6}$$

In which, X is a Design Matrix. W is a diagonal matrix with each entry represented by a separate weight function w that is same as Eq. 3.1. Y matrix is the y value of the observed data points [48]:

$$Y = \begin{bmatrix} y_0 \\ \vdots \\ y_n \end{bmatrix} \tag{3.7}$$

3.3.4 Diagnostics and Goodness of Fit

No single diagnostic technique can be used to determine the validity of the local regression. This requires a combination of diagnostic tools and studying them in conjunction with both the fitted values and the observed data. Several tools are usually used to evaluate the goodness of fit. First is the residual, the difference between observed and fitted values. The second is the fitted degrees of freedom, characterizing the overall smoothing.

$$\begin{aligned} v_1 &= \sum_{i=1}^{n} \mathrm{infl}(x_i) = tr(L) \\ v_2 &= \sum_{i=1}^{n} \left\| l(x_i) \right\|^2 = tr(L^T L). \end{aligned} \tag{3.8}$$

where L is the hat matrix [48]:

$$\begin{pmatrix} \hat{\mu}(x_1) \\ \vdots \\ \hat{\mu}(x_n) \end{pmatrix} = L \cdot Y. \tag{3.9}$$

The prediction mean squared error (PMSE[48]) is also useful in assessing the performance of the fit [48]:

$$PMSE(\hat{\mu}) = E(Y_{new} - \hat{\mu}(x_{new}))^2 \tag{3.10}$$

$PMSE(\hat{\mu})$ depends on assumptions made about x_{new}. For now, assume that the design points $x_1,...,x_n$ are independent samples from a density $f(x)$, and the new point x_{new} is sampled from the same density. The cross validation method provides an estimate of PMSE. The cross validation estimate of the PMSE of an estimate $\hat{\mu}$ is [48]

$$CV(\hat{\mu}) = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{\mu}_{i-1}(x_i))^2 \tag{3.11}$$

Where $\hat{\mu}_{i-1}(x_i)$ denotes the leave -x_i- out estimate of $\mu(x_i)$. That is, each x_i is deleted from the dataset in turn, and the local regression estimate computed from the remaining *n-1* data points.

The generalized cross validation (GCV) criterion is introduced to provide an approximation of PMSE. GCV score for a local estimate $\hat{\mu}$ is

$$GCV(\hat{\mu}) = n\frac{\sum_{i=1}^{n}(Y_i - \hat{\mu}(x_i))^2}{(n-\nu_1)^2} \tag{3.12}$$

where ν_1 is the fitted degrees of freedom defined by Eq. 3.8. However, Cleveland and Devlin argued that GCV score discards much information about the bias-variance trade-off that the statistics provide. Therefore, they introduced the GCV plot [39]. A GCV plot uses the fitted degrees of freedom $tr(L^T L)$ as the horizontal axis and the GCV score as the vertical axis. By trading-off the degrees of freedom and GCV score, it is easy to find an appropriate smoothing parameter from the GCV plot and fit the data set well.

As a summary, in Step 4 of the computational infrastructure of the design exploration method for adaptive design systems, local regression surrogate models are developed to replace the computationally intensive original simulation models. In next step, the inverse manner design exploration method employs these surrogate models to find the best ranged set of solutions against the uncertainty.

3.4 DESIGN PROCEDURE OF INVERSE DESIGN EXPLORATION

3.4.1 Overview of the Inverse Design Exploration

The inverse design exploration is the core of the design exploration method for adaptive design systems, which is proposed to deal with the uncertainties from the control factors, noise factors and models themselves. The solution strategy is to find a ranged set of solutions in a top-down manner (inverse) in the model chain. In other words, the design process should start from the evaluations of the top level models to lower level models. Therefore, in the DEM-ADS, this top-down manner design exploration is called as the inverse design exploration process. The prospective solutions should be far from the desired response range or constraints boundary in order to be robust to uncertainty existing in the system.

Different from IDEM, in which discrete design exploration is used in the inductive design process and all of the feasible solutions are found as the set of solutions, the inverse design exploration in DEM-ADS implements efficient solutions search algorithm to find the set of solutions with the largest EMI. Because in the adaptive design systems, designers are able to obtain sufficient design information, the size of design freedom, or the number of feasible solutions, can be defined by designers. The discrete exploration is not necessary in the adaptive design. Due to the efficient solution search algorithms, the design exploration process of DEM-ADS must be efficient than IDEM. In this thesis, pattern search is chosen as the solution search algorithm.

The procedure for the proposed method is illustrated in Figure 3. 6. Input x is the design space and y is the intermediate space which is both the output of function y=f(x) and the input of function $z=g(y)$. z is the final response in this model chain. In the inverse design exploration process, a feasible ranged set of solutions in y-space is identified first with a response range satisfying design requirements in z-space, the desired response space. Then, the feasible y-space is treated as the desired response objectives for function $y=f(x)$, and then a feasible ranged set of solution in x design space can be achieved.

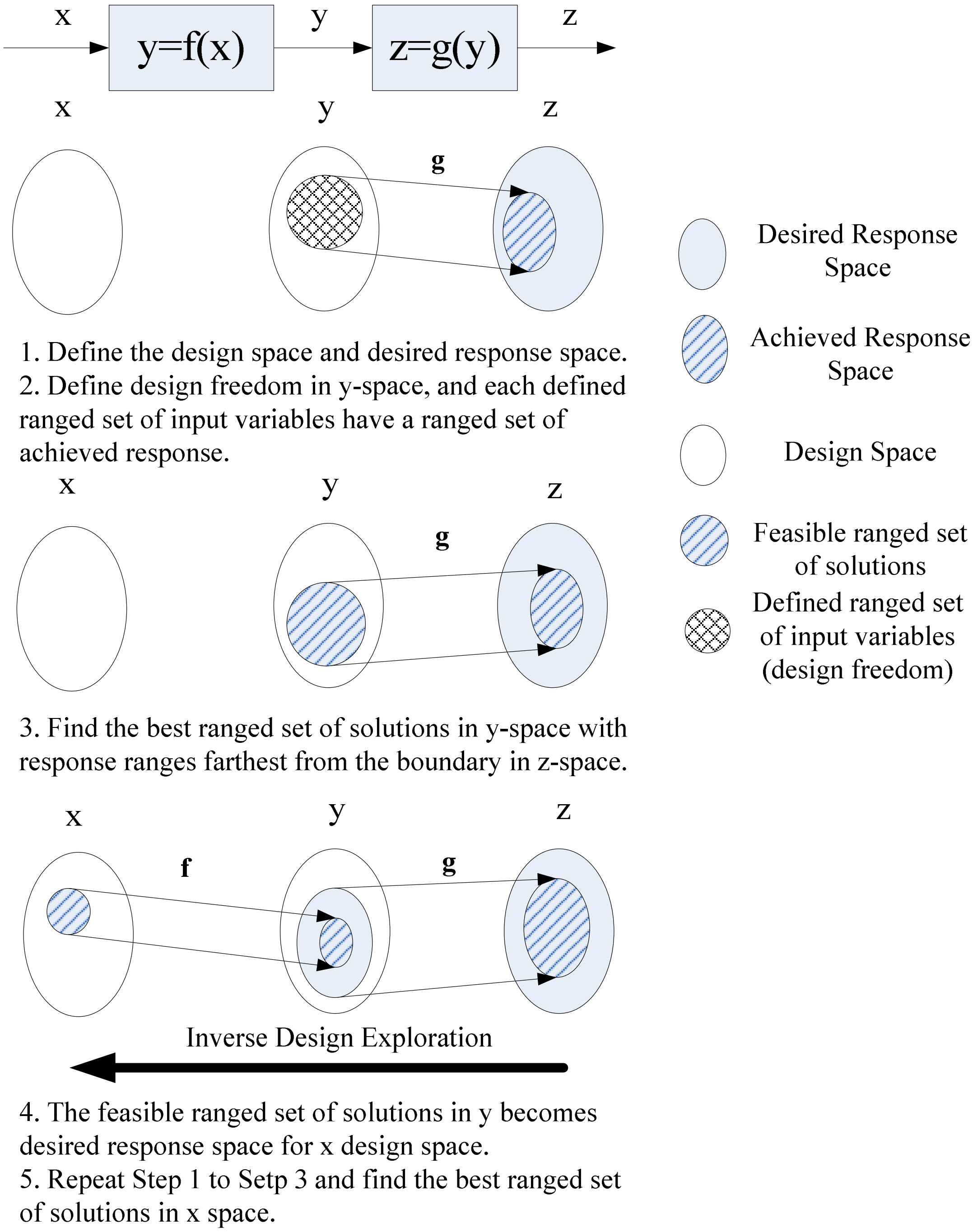


Figure 3. 6 - Inverse design exploration process

The procedure includes the following steps.

1. Design model chains are defined according to the system structure obtained in Step 1 of the design exploration method for adaptive design systems shown as Figure 3. 2. The design space (x-space and y-space in Figure 3. 6) and desired response space (z-space in Figure 3. 6) are identified according to the design variables bounds and design task objectives defined in the design task clarification in Step 2 of the proposed method.

2. The design freedom, is defined in y-space (intermediate space) according to the designers' expertise and design uncertainty condition. In this thesis, design freedom is defined as a ranged set of feasible solutions, in which designers have freedom to choose any solution from the set according to the designers' preference or other considerations. The size of design freedom can be defined by the "radius" of the solution range in terms of designers' preference, which is the absolute of the mean minus the maximum or minimum in the solution set. It is assumed that design freedom has a normal distribution.

$$dx = |x_{mean} - x_{Max}| \tag{3.13}$$

   Each ranged set of variable value in y-space have a ranged set achieved responses (achieved response space), which are obtained through response boundary exploration introduced in Section 3.4.2.

3. The achieved response space is evaluated by the Error Margin Index (EMI), introduced in Section 3.4.3. The ranged set of variable value in y-space associated with the achieved response space having the largest EMI is found as the feasible range set solutions in y-space.

4. The feasible ranged set of solutions in y-space becomes the desired response space for *f* function.

5. The feasible ranged set of solution in x-space is found in the same way as y-space. Step 1 to Step 3 of the inverse exploration process should be used again to find the best ranged set of solutions in x-space.

In this process, both inductive (top-down) and deductive (down-top) approach are implemented. In each design task, such as from y-space to z-space or from x-space to y-space, deductive approach is used because the mapping relationship is existing between the cause and effect because sufficient design information is available, which is different from material design problems. From the overall design process, the inductive approach is used in which the design process is solved from z-space to x-space. Therefore, this process is called as "inverse design exploration". The solution of the inverse design exploration is a ranged set of feasible solutions, instead of a single value solution. The design freedom is still available in the final solution, which can be against uncertainty or slight parameter modifications in further detail design.

In this inverse design exploration process, two important concepts should be used, response boundary exploration and the Error Margin Index (EMI). In the following two sections, these two concepts are introduced in details.

3.4.2 Response Boundary Exploration

The inverse design exploration procedure can be used for both response regression model, which can be represented as a mathematical function, and local regression model, in which an explicit mathematical function is not available. Different methods are used in the two cases.

In parametric cases, the response variance due to variations in the design variable vector, x, is obtained by first order Taylor series expansion. If the variations in input variables are assumed as small, the response variance is

$$\Delta Y = \sum_{i=1}^{n} \left| \frac{\partial f}{\partial x_i} \right| \cdot \Delta x_i \tag{3.14}$$

in which, n is the number of design variables. This representation of the response deviation is close to the worst case scenario, in which it is assumed that all fluctuations occur simultaneously in the worst possible combination [23]. However, this method still does not include the response variation due to the error or uncertainty from the model itself. As discussed in Section 2.1, in Type I-II-III robust design, model uncertainty is an important source of uncertainty.

Assuming a system model has 'n' uncertainty bounds, a response variation from each of them is obtained through [4]

$$\Delta Y_{\mathrm{j}} = \sum_{i=1}^{n} \left| \frac{\partial f_{\mathrm{j}}}{\partial x_i} \right| \cdot \Delta x_i \tag{3.15}$$

Where i=1, 2 … m, m is the number of design variables and j=1, 2 … n. The uncertainty bound functions can be either defined by designers or obtained from the confidence interval functions. Minimum and maximum responses caused by variability in m design variables and models with n uncertainty bounds are evaluated using [4]

$$Y_{\max} = Max\left\{ f_j(x) + \sum_{i=1}^{m} \left| \frac{\partial f_j}{\partial x_i} \right| \cdot \Delta x_i \right\} \tag{3.16}$$

And

$$Y_{\min} = Min\left\{ f_j(x) - \sum_{i=1}^{m} \left| \frac{\partial f_j}{\partial x_i} \right| \cdot \Delta x_i \right\} \tag{3.17}$$

where j=0, 1, 2 … n, $f_0(x)$ is the mean response model, $f_1(x)...f_n(x)$ are uncertainty bound functions and Δx_i is the "radius" of design freedom.

In nonparametric cases, such as local regression models used in this paper, instead of finding maximal and minimal responses boundary by Taylor series expansion, the efficient optimization method is employed to find out the maximal and minimal response boundaries within the design freedom, shown as Eq. 3.17.

If model uncertainty is not in the considerations, the maximal and minimal response within the specific design variable ranges can be found by the following functions:

$$Y_{\max} = \underset{x \in [xl, xu]}{Max} \{ f\ (x) \} \tag{3.18}$$

$$Y_{\min} = \underset{x \in [xl, xu]}{Min} \{ f(x) \} \tag{3.19}$$

where, xl is the lower boundary of the design range and xu is the upper boundary of the design range.

If model is taken into consideration, the uncertainty bounds should be used for response boundary exploration. 95% confidence intervals are applied as the uncertainty bounds for the non-parametric model. The minimal and maximal response boundary within the specific design variable ranges can be found by the following function:

$$Y_{\max} = \underset{x \in [xl, xu]}{Max} \{ f_{upper95\%}(x) \} \tag{3.20}$$

$$Y_{\min} = \underset{x \in [xl, xu]}{Min} \{ f_{lower95\%}(x) \} \tag{3.21}$$

3.4.3 Error Margin Index

In inverse design exploration, the Error Margin Index (EMI) is adapted to check the feasibility of the solution. In the inverse design exploration, only when all of the outputs are satisfactory, the output space is assumed to be feasible, so that any points in the design solution space can provide acceptable responses. By doing that, although the design freedom in the proposed method is reduced, the robustness of all feasible solutions increases. All solutions in the feasible ranged set can always have feasible and robust performance to uncertainty. All solutions with feasible response have the EMI larger than the one. The ranged set of solutions with the largest EMI is the solution for the inverse design exploration. For example, in Figure 3. 7, only one rectangle in the lower left square is feasible, because all of points around the mean are in the feasible range.

The summary of the EMI calculation is shown in Table 3. 2. The calculation of the EMI in inverse design exploration is similar to the EMI in the RCEM-EMI, discussed in Section 2.1.4. For most design problems, there are three design scenarios, “smaller response is better”, “larger response is better” and “nominal response is better”. In first scenario, an upper requirement limit (URL) is defined to represent the response constraints. In second scenario, a lower requirement limit (LRL) is defined to represent the response constraints. In third scenario, there is a target response defined in the design requirement. Both URL and LRL are defined in terms of the response constraints. EMI is calculated according to different scenarios. In order to obtain satisfying solution, EMI should be larger or at least equal to the unit, which means all of the points can provide a satisfactory response. The diagram construct of EMI is shown in Figure 3. 8, in which all responses are assumed to be normal distributions.

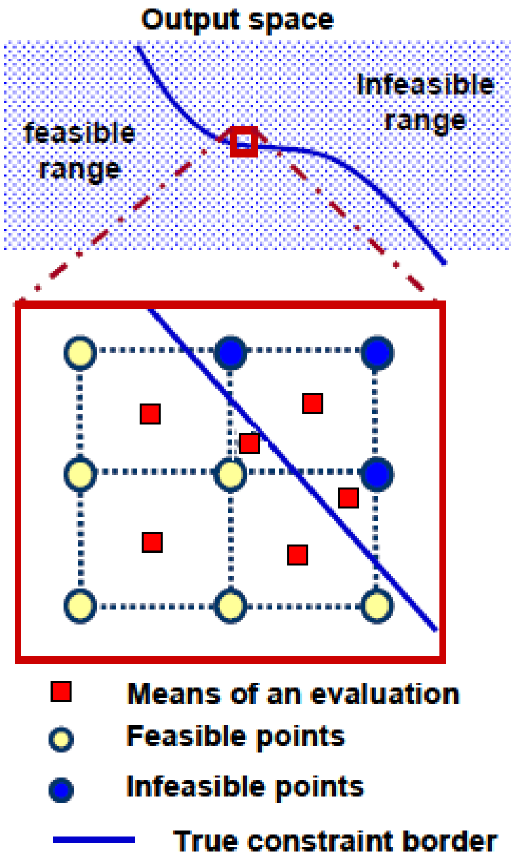
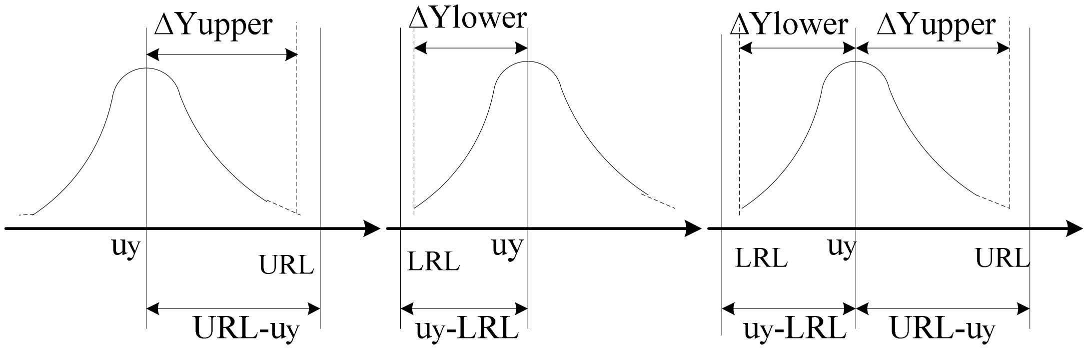


Figure 3. 7 - Feasibility evaluation technique [4]

Table 3. 2 - Calculations of EMI

$\Delta Y_i = Max\{(Y_{\max i} - mean_i), (Y_{\min i} - mean_i)\}$	
$EMI_i = \left\{ \dfrac{\lvert mean_i - LRL \rvert}{\Delta Y_i} \right\}$	(for larger is better, if all points are in feasible space)
or, $EMI_i = \left\{ \dfrac{\lvert mean_i - URL \rvert}{\Delta Y_i} \right\}$	(for smaller is better, if all points are in feasible space)
$EMI_i = Min\{ \dfrac{\lvert mean_i - URL \rvert}{\Delta Y_i}, \dfrac{\lvert mean_i - LRL \rvert}{\Delta Y_i} \}$	(for nominal is better, if all points are in feasible space)
where, i=1,2,…, number of response,	
$mean$	the mean value of the output of i th response
$Y_{\max}$	the maximum value of the response

Y_{min}	the minimum value of the response
ΔY	the largest distance from the mean of response
LRL	lower boundary of the response
URL	upper boundary of the response



（a）Smaller is better （b）Larger is better （c）Nominal is better

Figure 3. 8 - Diagram construct of Error Margin Index (modified from [4])

In the first design scenario, the design objective is to minimize the response, in other words, to keep response distribution away from *URL* as far as possible. *EMI* is calculated as Eq.3.20. The response range is satisfactory only when the maximum of the response range is smaller than the *URL*. The larger *EMI* means the response distribution is farther from the *URL*.

$$EMI = (URL - \mu_y) / \Delta Y_{upper}$$
$$EMI > 0 \tag{3.22}$$
$$where\ \Delta \mathrm{Y}_{upper} = Y_{upper} - \mu_y$$

In the second design scenario, the design objective is to maximize the response, in other words, to keep response distribution away from *LRL* as far as possible. *EMI* is calculated using Eq. 3.21. The response range is satisfactory only when the minimum of the response range is larger than the *LRL*. The larger *EMI* means the response distribution is farther from the *LRL*.

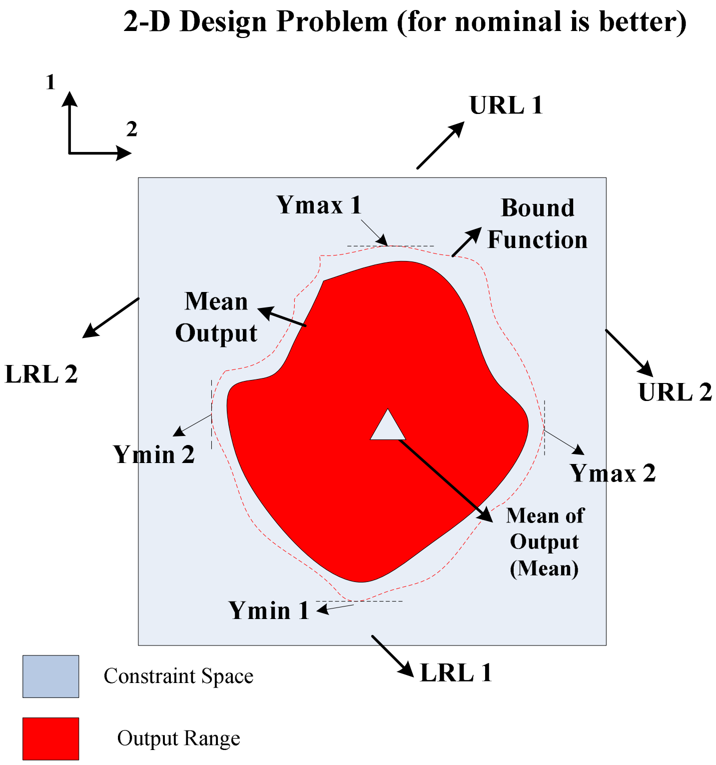
$$
\begin{aligned}
&EMI = (\mu_y - LRL) / \Delta Y_{lower} \\
&EMI > 0 \\
&where\ \Delta \mathrm{Y}_{lower} = \mu_y - Y_{lower}
\end{aligned} \tag{3.23}
$$

In the third design scenario, the design objective is to make the response close to a specific value. In this case, the response distribution should be kept away from both *URL* and *LRL* as far as possible. *EMI* is calculated as Eq. 3.22. The response range is satisfactory only when the minimum of the response range is larger than the *LRL* and the maximum of the response range is smaller than the *URL*. The larger *EMI* means the response distribution is closer to the middle of the space with *LRL* and *URL* as boundary.

$$
\begin{aligned}
&EMI = Min[EMI_l, EMI_u] \\
&where, \\
&EMI_l = (\mu_y - LRL) / \Delta Y_{lower} \\
&EMI_u = (URL - \mu_y) / \Delta Y_{upper} \\
&EMI > 0 \\
&\Delta \mathrm{Y}_{upper} = Y_{upper} - \mu_y \\
&\Delta \mathrm{Y}_{lower} = \mu_y - Y_{lower}
\end{aligned} \tag{3.24}
$$

In the multi-objective design problem, the *EMI* in each output direction has an individual value. EMI_i, defined as the *EMI* in *i*th direction, is the distance from the mean of the output space to the target value (mean of the constraint space) in *i*th direction. As *EMI* values decrease, the output ranges move closer to the target in constraint space.

In Figure 3. 9, the output space is two-dimensional and the feasible region in the output space is described as a contour (constraint boundary) with upper and lower boundaries. The dark regions represent an output range with a mean value in its center. The dashed contour represents the interval boundary of this 2-D output. The critical values are shown in the figures, as Y_{min} and Y_{max}. In the case shown in Figure 3. 9, which is a problem in which there is a specific target value, the output needs to be as far away as possible from the upper and lower boundaries. It depends on designers' preference to decide how to weight two objectives in the solution search exploration. In the next section, the compromise Decision Support Problem is introduced to formulate the design problem.



$$\Delta Y_1 = Max\left\{(Y_{\max 1} - mean_1),(Y_{\min 1} - mean_1)\right\}$$

$$EMI_1 = Min\{\frac{|\,mean_1 - URL_1\,|}{\Delta Y_1},\frac{|\,mean_1 - LRL_1\,|}{\Delta Y_1}\}$$

$$\Delta Y_2 = Max\left\{(Y_{\max 2} - mean_2),(Y_{\min 2} - mean_2)\right\}$$

$$EMI_2 = Min\{\frac{|\,mean_2 - URL_2\,|}{\Delta Y_2},\frac{|\,mean_2 - LRL_2\,|}{\Delta Y_2}\}$$

Figure 3. 9 - Example of two-dimensional EMI calculation (mathematical relationships)

3.4.4 Compromise Decision Support Problem (cDSP) for the Inverse Design Exploration

Inductive design exploration procedure uses the compromise Decision Support Problem (cDSP) to formulate the solution search. The cDSP provides a mean for solving multi-objective and non-linear design problems [17]. The cDSP is the mathematical construct through which the conflicting robust design goals in robust design traded off. The compromise DSP is used to find out the best solution spaces, shown as Table 3. 3.

Table 3. 3 - Compromise DSP in the EMI for robust design under uncertainty in design variables and models

Given

Mean Response functions, $f_i(x)$ where $(i=1,...,n), x=\{x_1, x_2, ..., x_m\}$

where *n* is the number of responses and *m* is the number of design variables;

Upper/ lower boundary functions, f_i^{upper} or f_i^{lower}, *i* is the number of the mean response functions;

System Constraints, $g(x)$

where *z* is the number of constraints;

Error Margin Indices:

$EMI = (URL - f_i(x)) / \Delta Y_{upper}$ for minimization problem;

$EMI = (f_i(x) - LRL) / \Delta Y_{lower}$ for maximization problem;

$$EMI_i = Min\{\frac{|f_i - URL|}{\Delta Y_i}, \frac{|f_i - LRL|}{\Delta Y_i}\}$$

$$\Delta \mathrm{Y}_{upper} = Y_{upper} - \mu_y$$

$$\Delta \mathrm{Y}_{lower} = \mu_y - Y_{lower}$$

Target performance and target of *ith* goal: EMI_i.

Find

The location of the mean of the input design space x_i, i.e., the design variables locations;

Deviations d_i^+, d_i^-.

Satisfy

	Goals: $EMI_i + d_i^+ + d_i^- = 0$ ($i = 1, 2, ...,$ Number of the goals)
	Bounds: $a_i \le x_i \le b_i$
	Constraints:
	$EMI_i > 0$
	$d_i^-, d_i^+ \ge 0$
	$d_i^- \cdot d_i^+ = 0$
Minimize	Deviation Function $Z = \sum_{i=1}^{n} [w_i (d_i^+ + d_i^-)]$
	where $\sum_{i=1}^{n} w_i = 1$

3.4.5 Computational Framework of Solution Search in DEM-ADS and IDEM

In the design exploration method for adaptive design systems (DEM-ADS), efficient solution search algorithm can be implemented in the solution search to replace the discrete design exploration, so that the efficiency of solution search can be improved. The computational frameworks of DEM-ADS and IDEM are compared in this section.

In the computational framework of DEM-ADS, the design freedom of each design variables, design bounds, and deviation functions are three inputs of the solution search algorithm. The deviation function can be obtained from the EMI calculation functions. All the input information of the solution search algorithm is defined in the compromise DSP which is discussed in Section 3.4.4. The solution search algorithm used in this thesis is the pattern search algorithm, which is introduced in Section 2.3.2. The pattern search is used to find the solution with minimum deviation function. The solution obtained is the set of solutions of the adaptive design system problem.

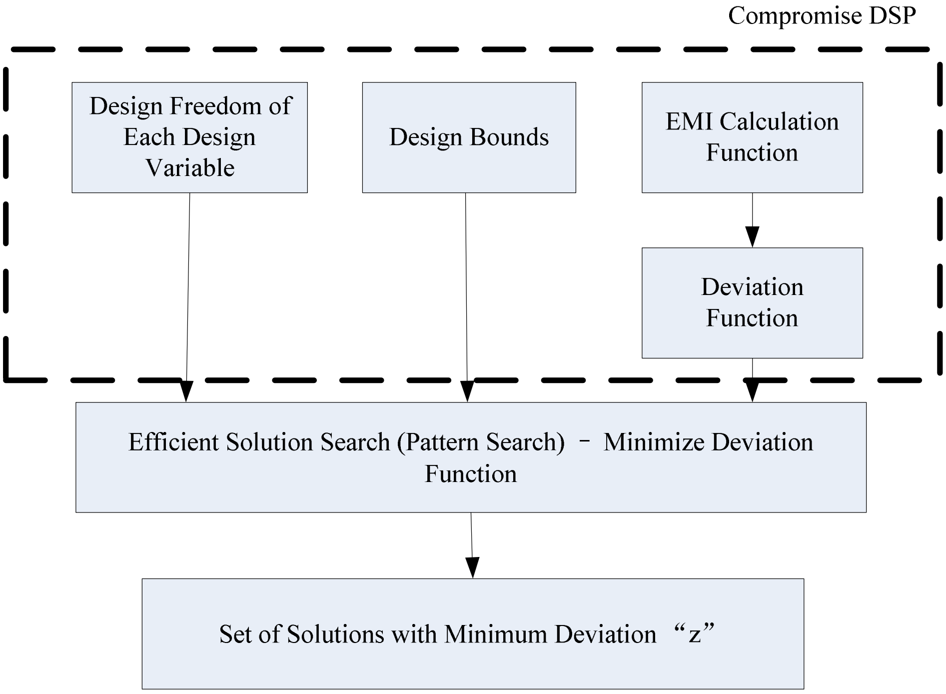


Figure 3. 10 Computational framework of solution search in DEM-ADS

Different from DEM-ADS, no efficient solution search algorithm is implemented in IDEM. The discrete design exploration, which is similar to the exhaustive solution search, is calculated based on step size of each design variable, design bounds and EMI calculation functions. The output of the discrete design exploration is the data set which includes all discrete points with EMI values. Then designers should define the satisfactory EMI value according to the robustness of solutions and the number of feasible solutions. Because the number of feasible solutions decreases when EMI value increases, the robustness of solutions and the number of feasible solutions should be compromised. In the IDEM, the compromise DSP is implemented in this step and satisfactory EMI value is defined to find out all feasible solutions. The ranged set of solutions with satisfactory EMI values is the solution of the adaptive design system problem. Therefore, the major computational framework is based on the exhaustive solution search. The IDEM is not an efficient design method.

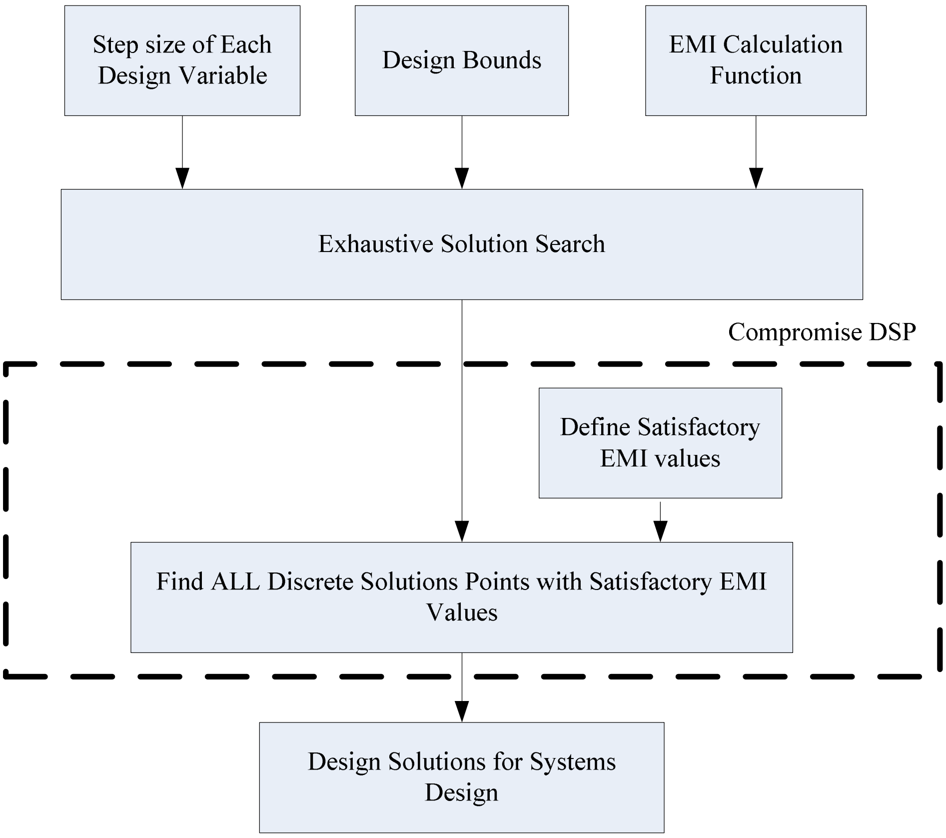


Figure 3. 11 Computational framework of solution search in IDEM

3.4.6 Robustness Analysis

The definition of the robustness is similar to that in the IDEM, since the inverse design procedure is modified from the IDEM. Unlike the Type I and Type II robust design, the objective in the proposed method does not focus on minimizing variations of model responses but keeps the responses always within the desired range under uncertainties. The solutions obtained from the proposed method has the largest *EMI* values, which means that responses can always be feasible even if the design variables vary due to the uncertainty and uncertainty propagation in the model chain. An example of the robustness of a solution obtained in Figure 3. 6 is shown in Figure 3. 12.

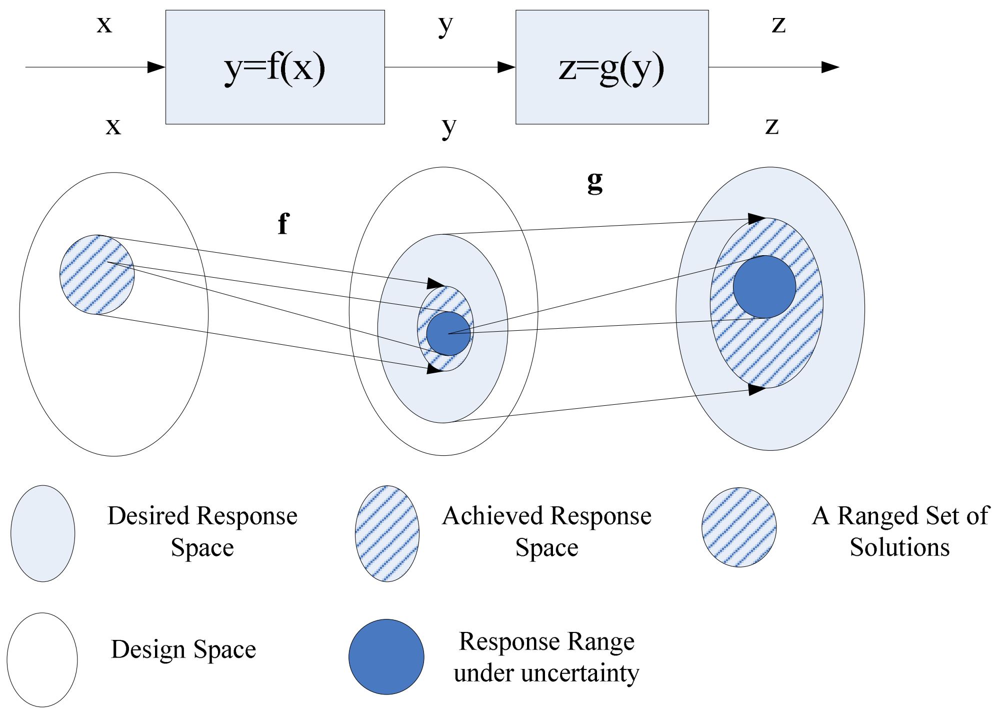


Figure 3. 12 - Robustness analysis of the inverse design process

As shown in Figure 3. 12, a ranged set of solutions have been achieved through an inverse design exploration process shown in Figure 3. 6. It is assumed that one solution in x-space is chosen by a designer from the ranged set of solutions. Due to the design variable uncertainty and model uncertainty, there is a response range associated with this solution in y-space. This response range must be within the achieved response space in y-space, which means that the responses are feasible in terms of design requirements. Since *y* is the intermediate design variable in this system design, it is also the design input variable of *g* function. One solution in y-space is chosen by the designer from the *y* response range. Due to the uncertainties in the system, the solution in y-space also has a response range in z-space. This response range must be also within in the achieved response space in z-space, which means that the responses are feasible in terms of design requirements. Therefore, all solutions in the ranged set of solutions are robust to the uncertainties in the system and the associated responses are in desired response range.

3.5 COMPUTATIONAL FRAMEWORK OF DEM-ADS

The DEM-ADS can be realized by different kinds of computational frameworks with different computational programs. In this thesis, the computational framework of DEM-ADS is illustrated in Figure 3. 13.

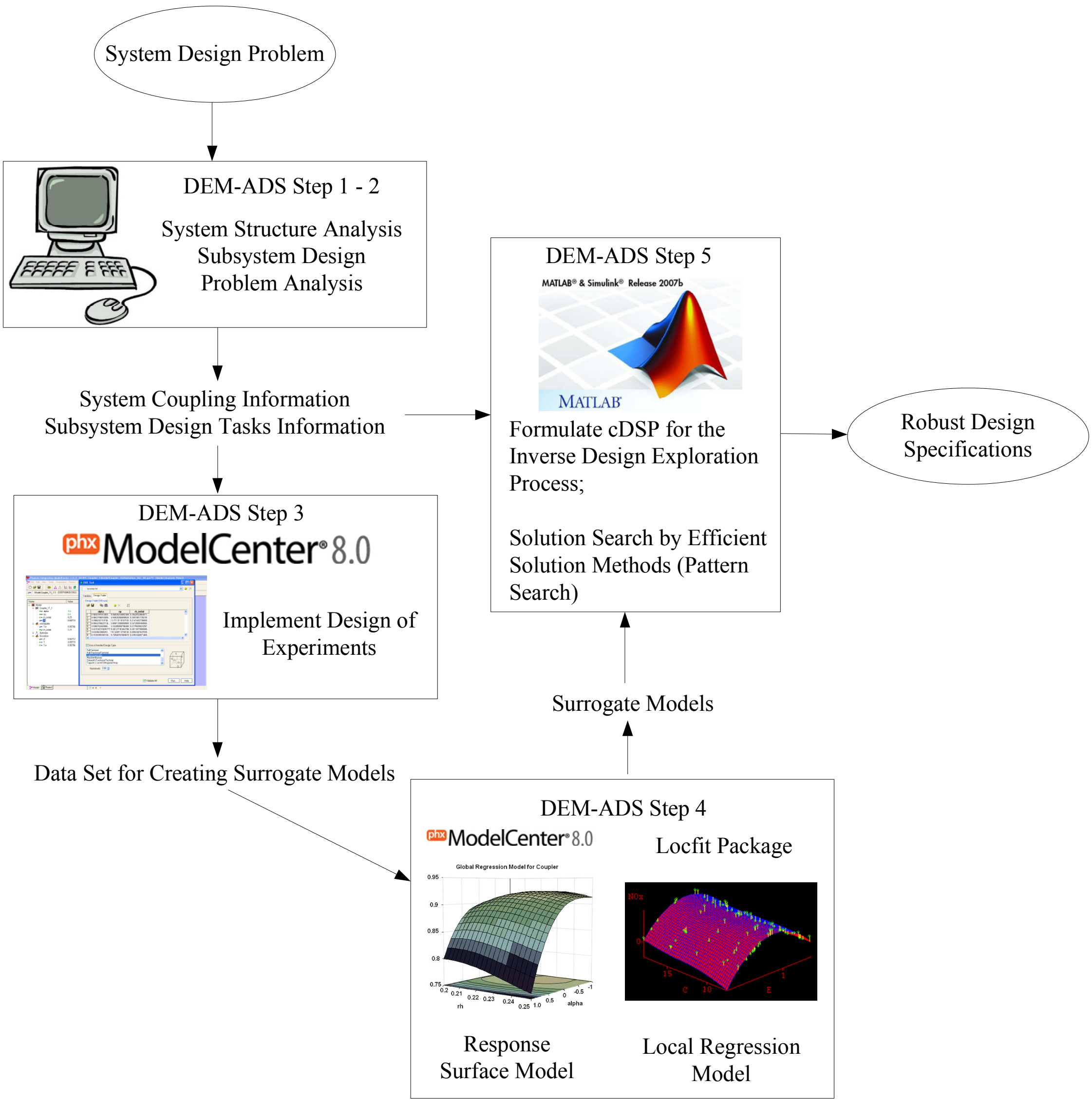


Figure 3. 13 - Computational framework of DEM-ADS

The computational framework shown in Figure 3. 13 shows how to realize each step in DEM-ADS in computer. The initial input of the computational framework of DEM-ADS is the design requirements, including the system design objectives and system models and the output of the framework are the robust design specifications.

DEM-ADS Step 1 – 2: The system design information is input into the computer, such as by SysML, or manually processed by designers if the design problem is not too complicated, such as in this thesis. In this step, system structure and coupling information is achieved, and each subsystem design task is identified. The coupling information is essential to define an inverse design exploration process in DEM-ADS Step 5, and the information of each subsystem design task is necessary to run Design of Experiments and create surrogate model in DEM-ADS Step 3 and Step 4.

DEM-ADS Step 3: In order to reduce the computational cost of the design process, the Design of Experiments and surrogate models should be established. In this computational framework, the ModelCenter is used to implement the Design of Experiments. In the ModelCenter, there are a lot of design types available, such as Full Factorial, Latin-Hypercube, and Taguchi 2 Level Orthogonal Array. Designers can choose appropriate methods for different subsystem models.

DEM-ADS Step 4: In this step, two surrogate models can be established according to different behaviors of model. As discussed in Section 3.3, if the model is not nonlinear, the response surface model is an appropriate method which is easy to use; if the model is highly nonlinear, the local regression model is appropriate to create more accurate surrogate model than the response surface model. ModelCenter, in this computational framework, is used to create response surface models and the Locfit package [56] is implemented to create local regression models. In the design solution exploration, designers work on the surrogate model obtained this step instead of the original simulation models.

DEM-ADS Step 5: The cDSP for the inverse design exploration process can be formulated and efficient solution search methods, such as pattern search used in this thesis, can be implemented to solve the design problem in Matlab. The pattern search algorithm is available in the Genetic Algorithm and Direct Search Toolbox of Matlab. Designers can also use Genetic Algorithm or other Direct Search methods if necessary, which are all included in this Matlab Toolbox.

The computational framework presented in this section is just one example of how DEM-ADS can be realized in computer. Designers can implement any available computer programs with similar functions in each step. For instance, the Locfit package can be replaced by more efficient and accurate programs if available.

3.6 VERIFICATION AND VALIDATION OF THE DESIGN EXPLORATION METHOD FOR ADAPTIVE DESIGN SYSTEMS AND LOCAL REGRESSION MODEL

In the following section, value is added to the verification and validation of the developed design exploration method developed for adaptive design systems. To begin, the domain-independent performance validity of the design exploration method for adaptive design systems and the local regression method are examined. This chapter adds value to the domain-independent structural validity of a design method. The domain-independent structural validity of a design method relates to its internal consistency and the strength, limitations of applicability of the proposed design exploration method for adaptive design systems, developed in Chapter 3. The validation square road map is illustrated in Figure 3. 14.

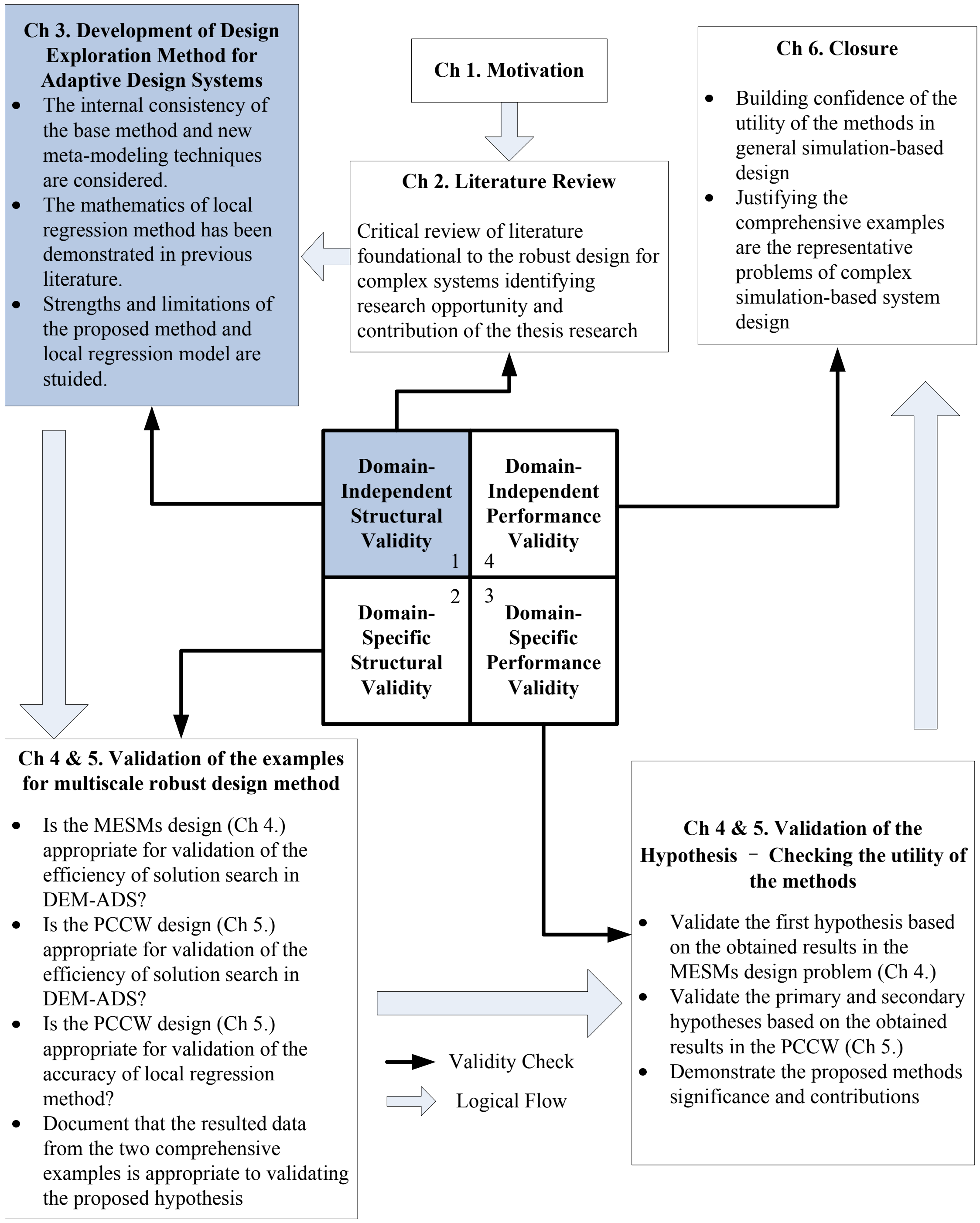


Figure 3. 14 - Validation square roadmap

A test for assessing the domain-independent structural validity of the design exploration method for adaptive design systems is in analyzing the information flow through the computing infrastructure to ensure that adequate input information is provided to each step, and adequate output information is provided for subsequent step. In Figure 3. 15, an information flow chart for the design exploration method for adaptive design systems is presented. As shown in the figure, all design information originates from the designers. Additionally, there are several decision nodes in the process requiring designer expertise information denoted in Figure 3. 15 with miniature designer icons.

As shown in Figure 3. 15, at the beginning of the process, a designer identifies basic design information, such as the system structure, system bounds and system design goals. This information serves as input information to the subsystem analysis and model response module in the inductive design exploration procedure. The subsystem analysis requires designers' preferences to determine the variables, preference, constraints, design bounds and design goals of each subsystem. Then, the information flows into the Design of Experiments to create samples. These samples flow into the model fitting module and designers should decide which model fitting method to be used to fit the samples. The output of the model fitting module is the information of surrogate mathematical subsystem models. In the design exploration method for adaptive design systems, both a response surface model and a local regression model can be used in this design stage. Since the local regression model introduced in this thesis has been widely applied as discussed in Section 2.2 and Section 3.3, and no modifications are made in this thesis, the internal consistency of local regression can be approved. The information, which outputs from the model fitting module, serves as input information to the inverse design exploration procedure. Because the internal information flow of the inductive design exploration procedure is based on the IDEM, thus, it follows that if the base method is internally consistent, then the proposed method is also internally consistent. The internal consistency of the base method is examined in detail in the Ph.D. dissertation of Hae-Jin Choi [4]. In Hae-Jin Choi's work, the domain-independent performance validity of the base method is tested by completing a conceptual example problem – the design of a cantilever beam and its associated material. Based on the effective application of the base method to the example problem, Choi asserts that IDEM is internally consistent. Therefore, the method in this thesis is internal consistent as well.

The output of the inverse design exploration procedure is the ranged set of robust solutions, and designers can choose the specific values from the solutions based on the preference and other considerations.

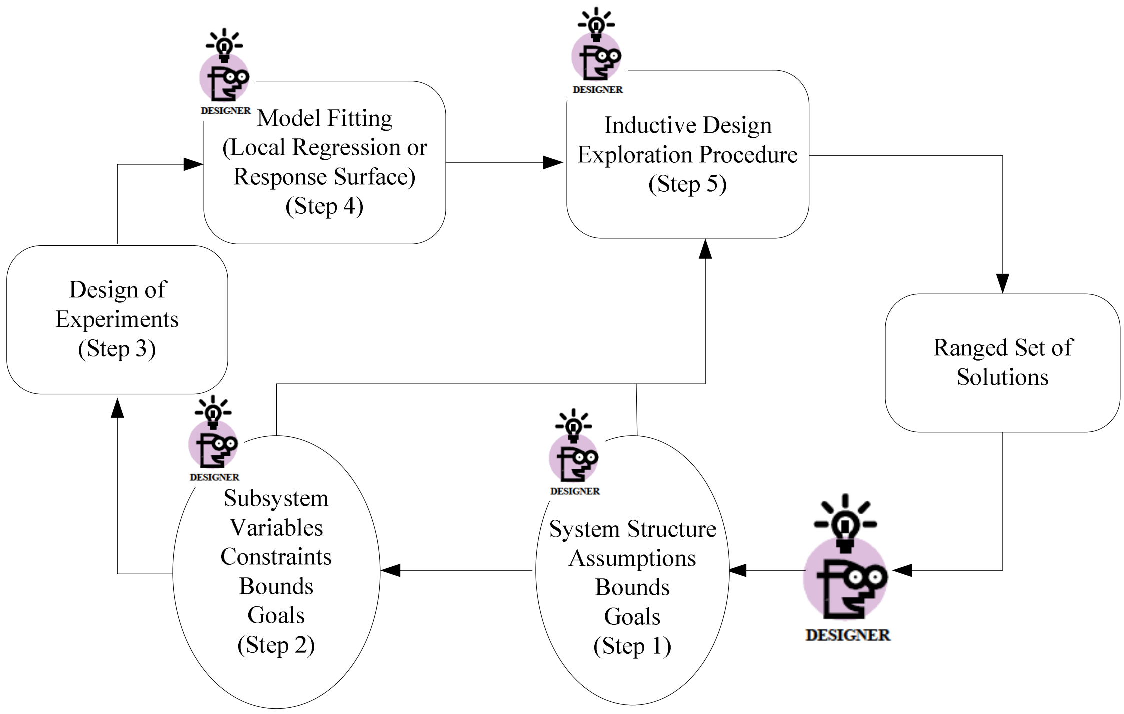


Figure 3. 15 - Information flow chart of the design exploration method for complex adaptive design

In addition, it is necessary to identify the strengths and limitations of proposed methods for the theoretical structural validity. The primary strength of the design exploration method for adaptive design systems is to improve the solution search efficiency in system design and find out robust solutions against uncertainty in the system. Because the design information, such as mapping relationship between inputs and outputs of analysis, is available, it is possible for designers to define design freedom and directly search the best ranged set of solutions instead of discretely exploring the whole design space. In addition, the proposed method also provides designers with design freedom against uncertainty or for parameter modification for further detail design. Moreover, due to the possibility of using continuous solution search methods in the inverse design exploration process, high computational costs, which are a serious limitation in the IDEM, are no longer a problem. It is possible to implement this method to a complex adaptive design systems problems in which the number of design variables in each systems are large. In addition, the proposed method makes the collaborative design possible. Because subsystem models are decoupled from the whole system design problem, it is possible for distributed designers to work on different design steps in sequence or in parallel, such as Photonic Crystal Coupler and Waveguide design problem in Chapter 5.

The primary limitation of the design exploration method for adaptive design systems is that the design freedom is smaller than IDEM. The small design freedom is reasonable only when design information is sufficient. Therefore, this method is specific for the adaptive and variant design. In the original design problem, the small design freedom may lead to a "no solution" situation.

Local regression modeling is proposed to improve the accuracy of surrogate models for nonlinear data. Response surface models, which are popular in engineering design, are difficult to fit nonlinear model accurately, unless high-order local polynomials are used. Local regression method is proposed to address this limitation. With its flexibility at fitting nonlinear data with different bandwidth, local polynomial degree or the weight functions, local regression method can either "honor the data" or "honor the trend". Therefore, although the local regression shows the same ability in fitting nonlinear data as kriging, it is better in the insensitivity to noise. The main limitation of local regression is that it is difficult to obtain the explicit regression function. Unlike the response surface model, which can be represented as a single mathematical function, the local regression model is a data set, including original sample data and local polynomials information. In order to exchange the regression model, designers may have to exchange all the DOE data and local regression program. In addition, since the explicit regression function is not available, the local regression may not be used in some design concept exploration programs which require regression functions as an input.

3.7 SYNOPSIS OF CHAPTER 3

The design exploration method for adaptive design systems presented in Chapter 3 provides the theoretical backbone for the reminder of the thesis. The proposed design approach is based on several key concepts from Chapter 2, such as robust design approaches, meta-modeling techniques and efficient solution search. The design exploration method for adaptive design systems is proposed to improve the efficiency of robust solution search against the uncertainty in systems. Local regression method is introduced into design process and proposed to improve the accuracy of surrogate nonlinear models and reduce model uncertainty in systems design. In order to complete the domain-independent structural validity, the advantages and limitations of the proposed methods are identified. In addition, the information flow is also examined. In this chapter, it is shown that DEM-ADS and local regression methods can address the research questions.

In next two chapters, Chapter 4 and 5, two appropriate design examples are solved by using the DEM-ADS and local regression methods to show the usefulness of the proposed methods. In Chapter 4, the MESMs design example is examined, which is to validate the primary hypothesis, DEM-ADS, in improving the efficiency of solution search compared to IDEM. In Chapter 5, the PCCW design example is examined, which is to validate both primary hypothesis and secondary hypothesis, in improving both the efficiency of solution search and accuracy of surrogate models. In Chapter 4 and Chapter 5, Domain-dependent Structural Validity and Domain-dependent Performance Validity are addressed.

CHAPTER 4
SIMULATION-BASED MULTIFUNCTIONAL ENERGETIC STRUCTURAL MATERIALS (MESMS) ROBUST DESIGN PROBLEM

In this chapter, the primary hypothesis is validated. In the primary hypothesis, the design exploration method for adaptive design systems is proposed to efficiently solve the systems design problems and control the propagation of uncertainties in the model chains. In Chapter 3, the implementation details including the overall procedure and the constituent techniques of the proposed method are discussed. In this chapter, a simple example, the simulation-based Multifunctional Energetic Structural Materials (MESMs) design example, is employed. The MESMs simulation and analysis models are logically connected and used for predicting the final response of the MESMs. This design problem was completed by Hae-Jin Choi in his Ph.D. dissertation [4]. The results of this example are supposed to show the advantages and usefulness of the DEM-ADS in improving the efficiency of solution search in adaptive design systems, by comparing the DEM-ADS solutions to the IDEM solutions.

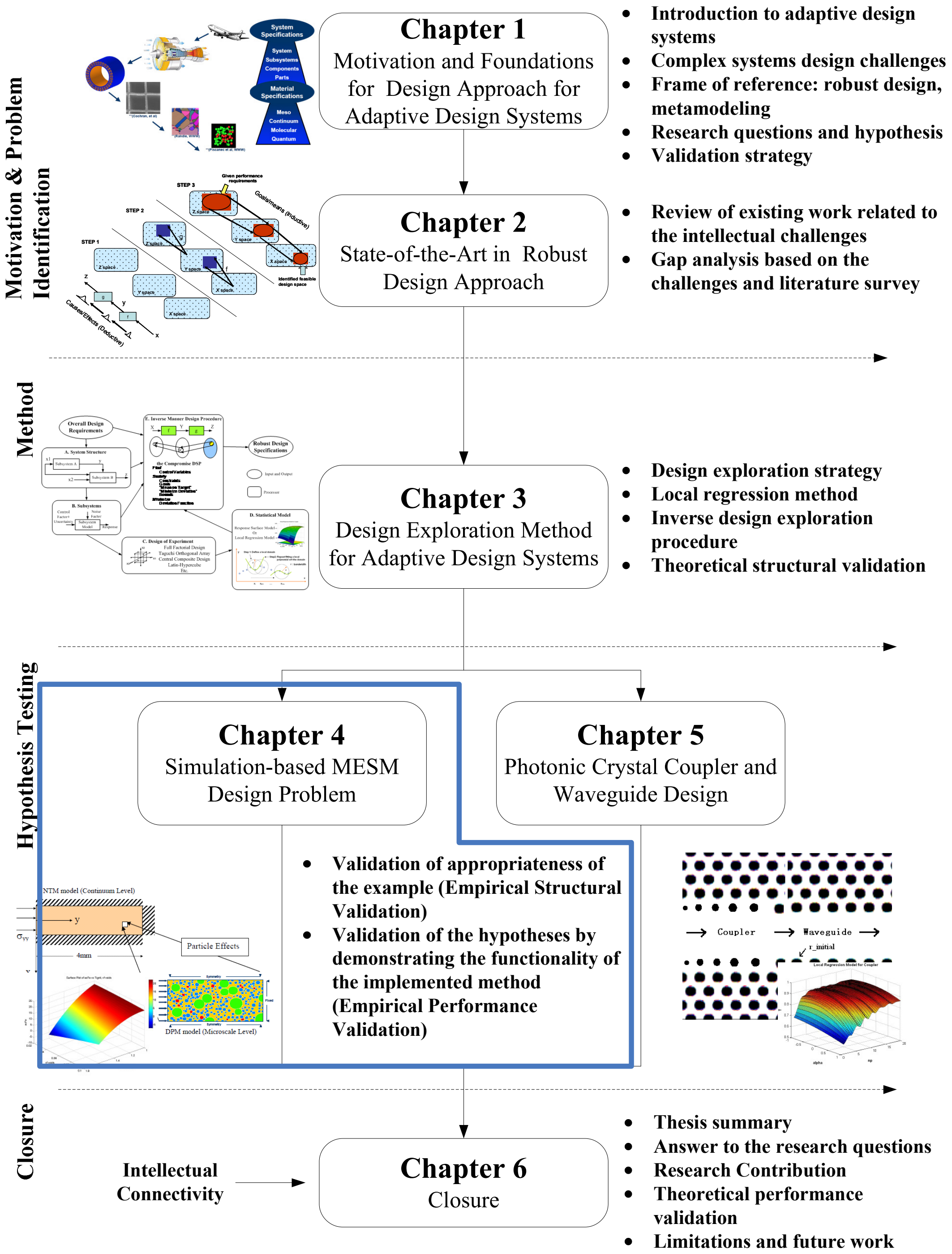


Figure 4. 1 - Thesis roadmap

In Section 4.1, the continuum level non-equilibrium thermodynamics mixture model and the microscale discrete particle mixture model are introduced. Two models are logically interfaced and formulate a simulation model chain. The value of completing this design problem is also addressed and this design problem is validated as an appropriate example for demonstrating the utility of the DEM-ADS, which is part of domain-specific structural validity in this thesis. In Section 4.2, the method is implemented to solve this design problem in detail. In Section 4.3, the IDEM solution obtained by Hae-Jin Choi is introduced and compared to the DEM-ADS. The comparison shows the advantage of the design exploration method for adaptive design systems. In Section 4.4, the solutions and hypothesis are validated by checking whether the DEM-ADS is useful for the MESMs robust design problem, which is part of domain-specific performance validity in this thesis.

4.1 INTRODUCTION OF THE SIMULATION-BASED MULTIFUNCTIONAL ENERGETIC STRUCTURAL MATERIALS DESIGN

In this section, a simulation-based MESMs design is introduced. This section is leveraged from Hae-jin Choi's PhD dissertation [4] with sight modification.

MESMs are multiphase mixtures of metal and metal-oxide, often with a binder phase. A candidate MESM system is micron scale $Al+Fe_2O_3$ particle mixtures with epoxy binder. A complementary design scenario discussed in this thesis is to tailor Al and Fe_2O_3 particle size and volume fractions, as well as the void volume fraction and mean void size, to maximize the total amount of chemical reaction for given shock loading conditions [13]. The complex simulation-based design is composed of the microscale Discrete Particle Mixture (DPM) model and the continuum level Non-equilibrium Thermodynamics Mixture (NTM) model developed by Lu and coauthors [49].

4.1.1 Non-equilibrium Thermodynamics Mixture (NTM) Model-Continuum Level

In this section, the Non-equilibrium Thermodynamics Mixture (NTM) model is briefly introduced, and the details of NTM model can be found in [49]. In this continuum level analysis, shock-induced chemical reactions in aluminum and iron-oxide mixtures are modeled in the frameworks of non-equilibrium thermodynamics and continuum mechanics, in which both the thermo-chemical and mechanic-chemical processes are accommodated. The constitutive model and conservation equation are formulated by introducing a combination of internal state variables and extended irreversible state variables. The internal state variables are mass fractions of reactants and products, and void contents. The extended irreversible state variables include chemical reaction rate, heat flux, and pore collapse flux. The irreversibility of these processes is implied in the nonnegative entropy production rate (i.e., the second law of thermodynamics) and their contribution to the dissipation. The relaxation time due to the duration of the chemical initiation and sustained reactions is in the range of 100-200 nano-seconds. A uniformly blended mixture theory is used to describe the porous mixture. The chemical reaction of the constituents is described as

$$2Al + Fe_2O_3 \rightarrow 2Fe + Al_2O_3 \tag{4.1}$$

The conservation equations, constitutive models, and chemical reaction equation, are described in detail in [49]. In this thesis, a one dimensional strain problem is implemented in Matlab, developed by Hae-Jin Choi [4]. The example is shown in Figure 4. 2. The top, bottom, and right boundary condition are fixed and initial loading (σ_{yy}) is applied on the left boundary. In this analysis, the amount of chemical reaction in the material system should be focused on. In order to assess the amount of chemical reaction, the mass fraction of Fe is the parameter to be captured since it is the product of the chemical reaction as shown in Eq. 4.1. In this study, we calculate the sum of the predicted mass fraction of Fe at all nodes in the finite difference meshes in the NTM model at 300 nano-seconds after the initial loading. This parameter is called the accumulated mass fraction of Fe (*acFe*) in this thesis.

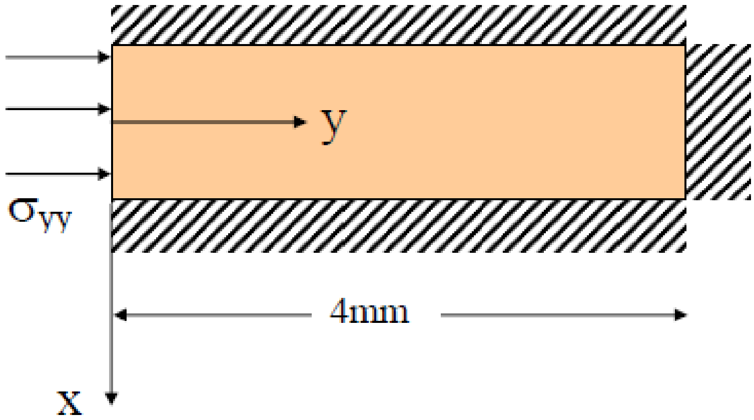


Figure 4. 2 - One dimensional shock simulation of Non-equilibrium Thermodynamics Mixture [4]

In summary, the NTM model is a non-equilibrium thermodynamic model incorporating shock-induced chemical reactions. In this model, void collapse flux, chemical reaction flux and heat flux and associated relaxation times in the constitutive models are included, which explains the delayed initiation and sustained chemical reaction. However, the reaction initiation conditions in the NTM model are assumed and these reaction initiation criteria need to be obtained from the lower scale model, the microscale Discrete Particle Mixture (DPM) model, to predict simulation results more accurately. For this reason, we need to formulate a multiscale analysis chain incorporating the microscale DPM model and the continuum NTM model in order to provide accurate reaction behavior of the Al and Fe_2O_3 mixture system.

4.1.2 Discrete Particle Mixture (DPM) Model – Microscale Level

The Discrete Particle Mixture (DPM) model is an explicit Eulerian finite element simulation that provides spatial resolution of the coupled thermal, mechanical, and chemical responses at the particle level during shock compaction. The details of the model are developed by Austin and co-authors .

In this model, shock waves are propagated through the particle system to characterize the thermo-mechanical conditions that lead to reaction initiation. Input parameters of this model are constituent particle size distributions (aluminum and iron-oxide), volume fractions, spatial arrangements or correlations of the particles in space, and shock strength on the overall thermal and mechanical responses of the material. The simulation is performed using the Eulerian hydrocode Raven, developed by Benson [6], with constitutive subroutines for the various phases developed by Austin and co-authors [4]. Pressure and temperature distributions are computed in a Statistical Volume Element (SVE) shown in Figure 4. 3 (a), at all stages of shock wave propagation, as shown in Figure 4. 3 (b). The DPM model is a computationally intensive, non-deterministic simulation with large amounts of random noise in the results due to the randomness of the simulated microstructure. This simulation work was done by Hae-jin Choi during his PhD study [1].

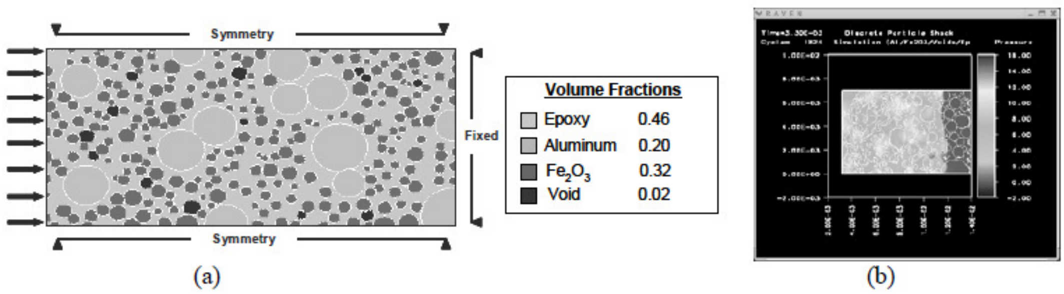


Figure 4. 3 - Microscale DPM model: (a) an SVE realization of the mixture model, and (b) simulated pressure distribution [13, 50]

4.1.3 System Design Analysis of Simulation-based MESMs Design

In this section, the multiscale coupling in this system design is identified between NTM and DPM models. This section is leveraged from Hae-Jin Choi's PhD dissertation [1].

The NTM model is based on a uniformly blended mixture theory ignoring the heterogeneity of discrete particles since it is too computationally intensive to include those discrete particles in a large domain. The reason for connecting the NTM and DPM models is including the discrete particle effects of the microscale level DPM model in the continuum level NTM model. As illustrated in Figure 4. 4, a SVE of the DPM model could be shown as a small square in the domain of the NTM model. The length of the NTM model specimen is round 4mm while the length of the SVE of the DPM model is 22μm.

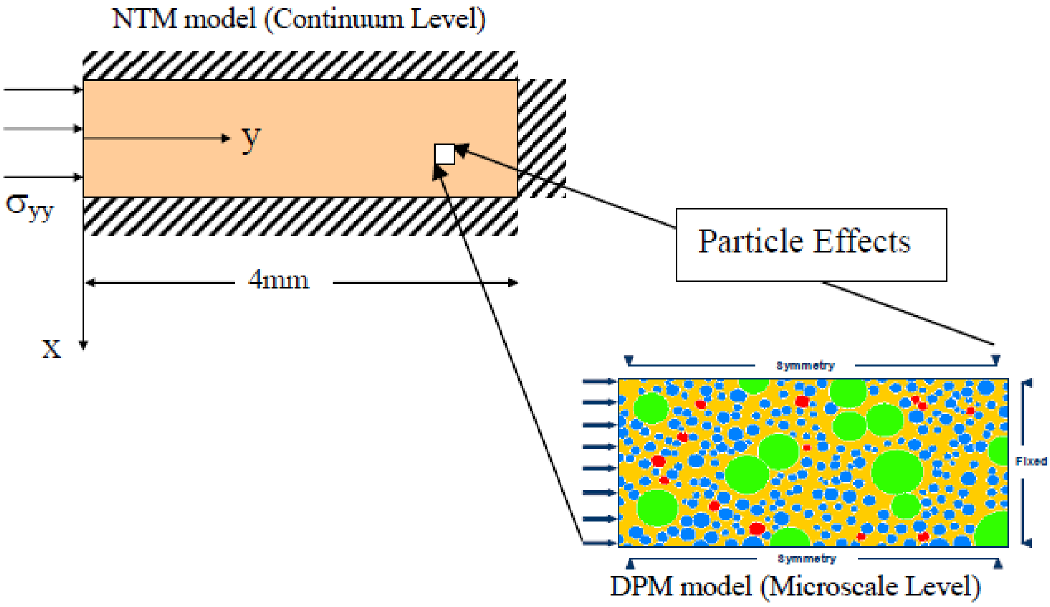


Figure 4. 4 - Complex MESMs system analysis model

The logical interface between the NTM model and DPM model is to characterize local reaction initiation conditions using the DPM model and then input the identified reaction initiation condition in the NTM model as a function of particle morphology and distribution. In this problem, temperature is assumed to be the main criterion for assessing initiation of chemical reaction. The hot spots where reaction is initiated are illustrated in a temperature distribution profile at the time when the first reaction starts, Figure 4. 5. The critical temperature initiating the chemical reaction is the average of the hot spot temperatures with weighting by the spot sizes. The weighted average temperature is the input parameter in the NTM model as the reaction initiation condition. The weighted average of temperatures of local hot spots at a first reaction initiation (T_{ignit}) is

$$T_{ignit} = \frac{\sum_{i=1}^{n} A_i \cdot T_i}{\sum_{i=1}^{n} A_i} \tag{4.2}$$

where n is the number of hot spots, T is the temperature of a hot spot, and A is the size of a hot spot.

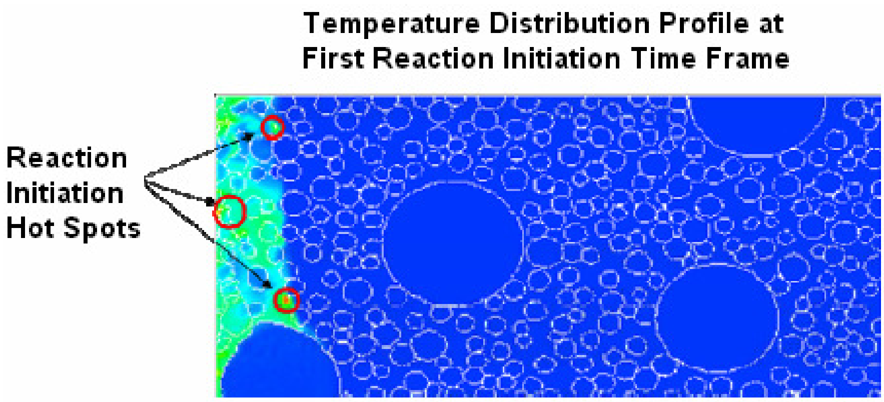


Figure 4. 5 - Local hot spots at a first reaction initiation time frame in the DPM model [4]

The obtained T_{ignit} in the DPM model is then used as the reaction initiation criterion in the NTM model as illustrated in Figure 4. 6.

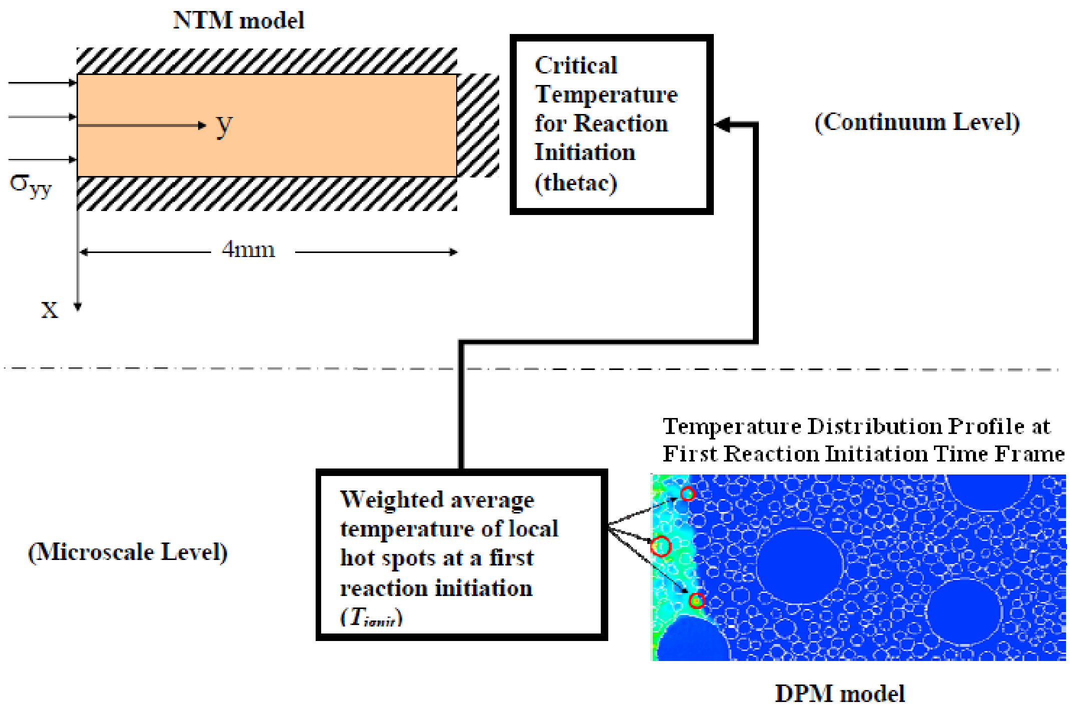


Figure 4. 6 - Connecting the NTM model and the DPM model [4]

4.1.4 Value in Completing the Simulation-based MESMs Design

Addressing Research Questions

The simulation-based MESMs design problem is selected because it is a system design problem with a multi-level coupling. This design problem is well defined and solved by Hae-jin Choi in his dissertation [4]. Therefore, in this design problem, it is not necessary to discretely explore the whole design space as the IDEM does. Although this problem is not adaptive design, it has a similar assumption: sufficient design information is available. The primary motivation in completing the MESMs design example problem is to demonstrate the usefulness of the DEM-ADS in efficiently finding a ranged set of solutions robust to the uncertainty in the model chain, which is the primary research hypothesis. The application of the DEM-ADS to the MESMs example problem, and the evidence of useful results, add value to the verification and validation of DEM-ADS presented in Chapter 3.

Verification and Validation of robust design approach for complex systems

Additionally, completing the MESMs design problem adds value to the verification and validation of the design exploration method for adaptive design systems. The MESMs example problem contributes to the domain-specific structural validity and the domain-specific performance validity of the proposed method. Additionally, the MESMs design problem is intended to illustrate the key advantages of DEM-ADS. One of the important advantages of DEM-ADS is the efficient solution search process, and it can be represented by the comparison of the design exploration efficiency of two methods.

4.2 SIMULATION-BASED MESMS DESIGN PROCESS AND SOLUTION

In the following section, the problem of MESMs design is presented. The design problem is solved by the design exploration method for adaptive design systems discussed in Chapter 3 and illustrated in details step by step. System structure of this design problem is analyzed and the coupling in this problem is identified. Then, each subsystem model is studied and uncertainty is identified. Meta-models are created for each subsystem model to save the computing cost and identify the model uncertainty based on the DOE results. Then inverse design exploration process is employed to find a ranged set of solutions. The successful implementation of the proposed method to the MESMs design problem builds confidence in the verification and validation of the method to the robust design of systems.

4.2.1 System Structure Analysis of MESMs Design Problem

Based on the logical interface discussed in Section 4.1, the system structure for designing MESMs based on the complex systems models is discussed in this section.

At the microscale DPM model, the input variables are the mean radius of Al particles, the mean radius of Fe_2O_3 particles, the volume fraction of voids, and the mean radius of voids. The output of the DPM model is the weighted average of the temperatures of local hot spots at first reaction initiation (*Tignit*). The simulation work was done by Hae-Jin Choi during his PhD study [1].

At the continuum NTM model, input variables are a critical temperature for chemical reaction initiation, which is also the output of the DPM model (T_{ignit}), and the volume fraction of voids, which is also the input of the DPM model (x3). The response that we capture from the NTM model is the accumulated mass fraction of Fe (acFe) over the entire one-dimensional specimen at 300 nano-seconds.

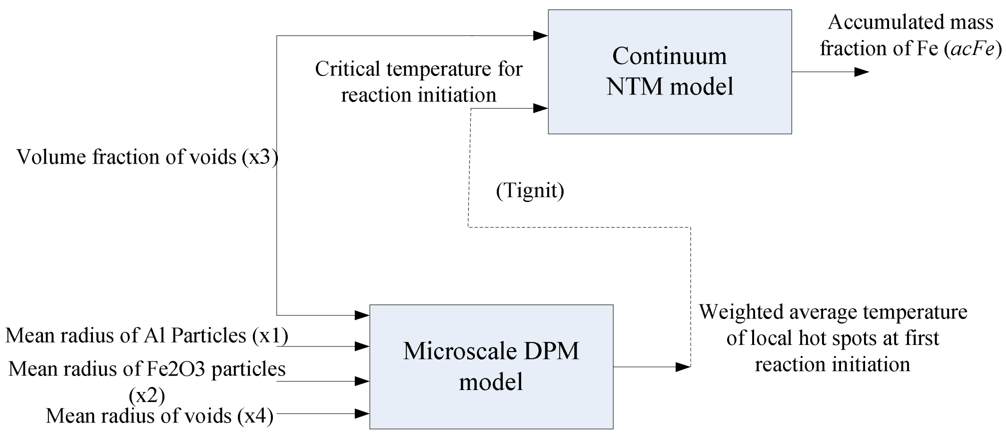


Figure 4. 7 - System structure of MESM design problem

The system structure of the MESM design problem is illustrated in Figure 4. 7. As shown in the figure, the volume fraction of voids is the shared input variable by the two models.

The output of the DPM model, the weighted average temperature of local hot spots at a first reaction initiation, is one of the inputs of the NTM model, critical temperature for reaction initiation, which is the interdependent variable.

4.2.2 Subystem Analysis

Since the MESMs design is complex and hierarchical, it is unreasonable to assume that the system model as deterministic – there are no random errors in a system response. In addition, uncertainty is associated with model-based prediction for some reasons. This section is leveraged from Hae-Jin Choi's PhD dissertation with modifications [4].

Uncertainty Analysis of DPM model

DPM simulation generates a distribution of varied outputs for the replication of a single input. The interval of the variation is from 1078K to 1697K. The mean output calculation has to depend on the metamodeling techniques. When the variances in design variables (*x1-x4*) are also considered, the uncertainty should become more significant. In addition, the model uncertainty in the DPM model should also be considered due to an uncertain constitutive model for iron-oxide and idealization from 3D particles to 2D cylinders.

Uncertainty Analysis of NTM model

NTM model contains the uncertainty caused by the variance in design variable x3 shared with the DTM model and the varied output of the NTM model. Besides them, NTM model also contains the uncertainty due to the assumptions made in this problem. The response employed in this design problem is a weighted average of the hot spot temperatures at the first reaction initiation. However, it is not fully validated that the average temperature in the DPM model is equivalent to the critical temperature for the chemical reaction initiation in the NTM model. The criteria for chemical reaction initiation derived from the microscale DPM model needs to be further investigated in order to include the delay in the chemical reaction. A major assumption in the NTM model is the uniformly blended mixture theory used for describing discrete particles and porous mixtures, which is a simplification for enabling numerical calculation in a larger scale continuous medium. This assumption could produce some unquantifiable uncertainty in responses, which requires a model calibration process based on real experimental results. This uncertainty could cause variations in the predicted response of *acFe*. There are the sources of model uncertainty discussed in Section 2.1.

As discussed in this section, the complex simulation-based MESM design task is associated with different sources of uncertainties. In the simulation chain, these uncertainties will be accumulated and propagated. Therefore, it is quite necessary to implement the robust design approach to solve.

4.2.3 Design of Experiments and Model Regression

For achieving an accurate regression model, a central composite design with two factors is employed in the NTM model study. This experiment was completed by Hae-Jin Choi during his PhD study. The experiment points and the NTM model analysis data are listed in Table 4. 1.

Table 4. 1 - Experimental points and obtained data using continuum NTM model code

Volume Fraction of Voids (x3)	Tignit (1000K)	acFe(responses)
0.032	1.088	19.452
0.088	1.088	21.615
0.032	1.512	0
0.088	1.512	8.975
0.02	1.3	12.892
0.1	1.3	16.776
0.06	1	22.054
0.06	1.6	0

As shown in Figure 4. 8, the regression parameters of a full quadratic response surface model of acFe versus *x3* (volume fraction of voids) and *Tignit* are estimated using Matlab. The full quadratic response surface model fits well with the obtained data (R-sq=99.2%). The mean response function of the NTM model is shown in Eq. 4.3.

$acFe_{mean} = f_0(x_3, T_{ignit})$: Response Surface Model

where $f_0(x_3, T_{ignit}) = 2.07 + 66.3 \cdot T_{ignit} - 271 \cdot x_3 + 287 \cdot x_3 T_{ignit} - 46.5 \cdot T_{ignit}^2 - 231 \cdot x_3^2$

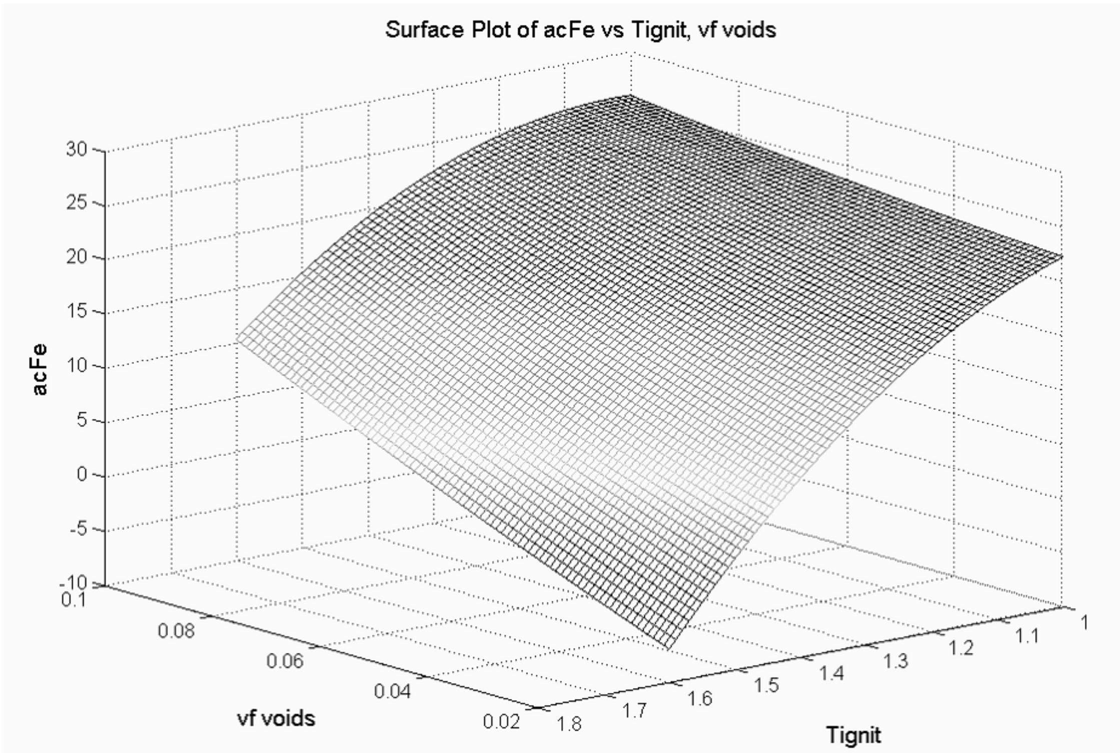


Figure 4. 8 - The estimated response surface of acFe versus x3 and Tignit

The Design of Experiments in DPM model was completed by Hae-Jin Choi during his PhD study. In the DOE, 360 simulation data points are collected using the simulation infrastructure [4]. The simulation data includes about 15 replicates at each experimental point. It is impossible to collect the responses from all performed simulations because the response is only achieved when a shock induced reaction is initiated. Hae-Jin Choi's regression model for the NTM model is acceptable and it is also used in this thesis.

A quadratic response surface model is employed as the mean response model and an exponential function powered by a quadratic response surface model is used as a conditional variance model. The estimated mean response model (y_{mean}) and the upper and lower bound of the prediction interval (y_{upper} and y_{lower}) are [4]:

$$
\begin{aligned}
y_{mean} &= (\hat{\beta}_{converged} \cdot x')^{-1/3} - 2 \\
y_{upper} &= \left\{ \hat{\beta}_{converged} \cdot x' - t_{N-P,1-\alpha/2} \cdot \exp\left(\frac{\hat{\beta}_{converged} \cdot x'}{2} \right) \right\}^{-1/3} - 2 \\
y_{upper} &= \left\{ \hat{\beta}_{converged} \cdot x' + t_{N-P,1-\alpha/2} \cdot \exp\left(\frac{\hat{\beta}_{converged} \cdot x'}{2} \right) \right\}^{-1/3} - 2
\end{aligned}
\qquad (4.4)
$$

where $x = [1, x_1, x_2, x_3, x_4, x_1^2, x_2^2, x_3^2, x_4^2, x_1 x_2, x_1 x_3, x_1 x_4, x_2 x_3]$ and

$\beta = [\beta_0, \beta_1, \beta_2, \beta_3, \beta_4, \beta_{11}, \beta_{22}, \beta_{33}, \beta_{44}, \beta_{12}, \beta_{13}, \beta_{14}, \beta_{23}, \beta_{24}, \beta_{34}]$.

The number of samples (*N*) is 360, the total number of predictors (*P*) is 30, and the confidence level ($1-\alpha$) is 0.99. The converged regression parameter for the mean response model is shown in the Table 4. 2. A sample estimated model is illustrated in Figure 4. 9.

Table 4. 2 - Converged regression parameter for the mean response model [4]

Subscripts	$\hat{\beta}_{converged}$
0	0.057632
1	1.0566
2	-41.796
3	-0.28438
4	-33.785
11	986.21
22	29929
33	1.9563
44	13711
12	2270
13	74.761
14	1351.5
23	-55.384
24	10091
34	195.5

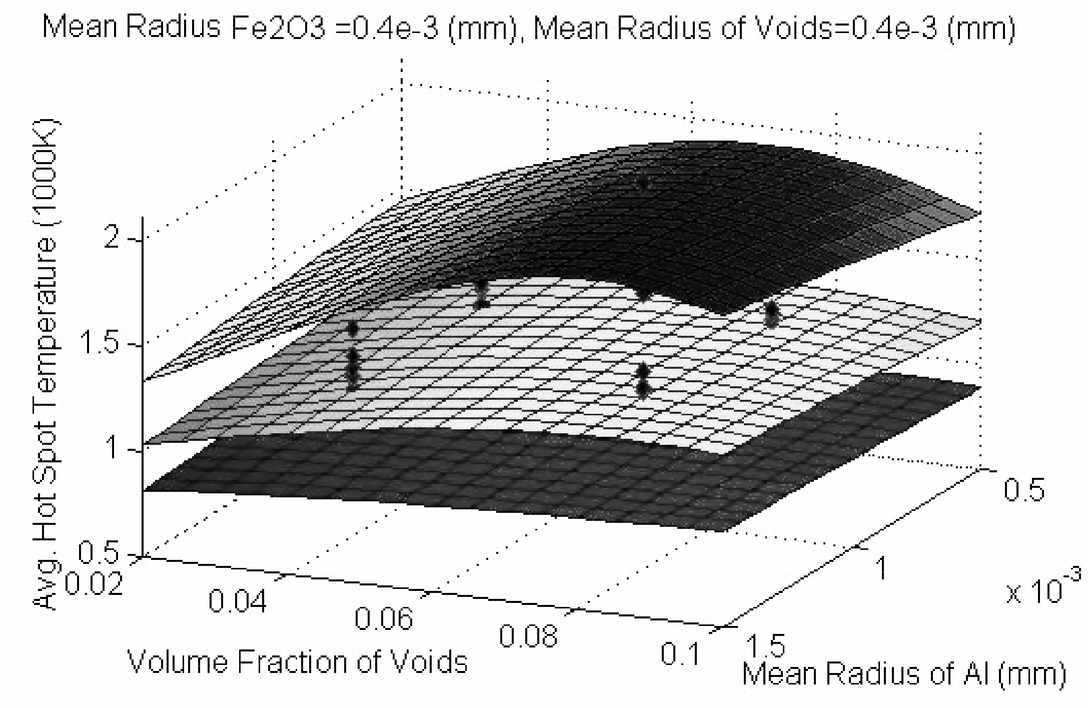


Figure 4. 9 - Estimated mean response model and upper/lower bounds of the prediction interval [4]

4.2.4 Inverse Design Exploration Procedure for MESMs Design Problem

The fifth step in DEM-ADS is to implement the inverse design exploration process to find ranged set of solutions against the uncertainty in the system. This design process is illustrated in Figure 4. 10. In terms of the system structure of MESMs design problem in Figure 4. 7, the design objective is to maximize the response (*acFe*), which is the output of the NTM model. The design procedure starts from NTM model. Therefore, the calculation starts from the NTM model. The best ranged set of solutions of NTM model can be found by maximizing the EMI. For DPM model, *Tignit* is the response, while x3 is one of the input variables. Therefore, the design range of *Tignit* obtained from the NTM model design becomes the design objective for DPM model, and the design range of *x3* obtained from the previous step becomes the design boundary of *x3* for the DPM model. After maximizing EMIs, the specific design ranges of DPM model can be found. As shown in Figure 4. 10, the design range of *x3* is further reduced after DPM design.

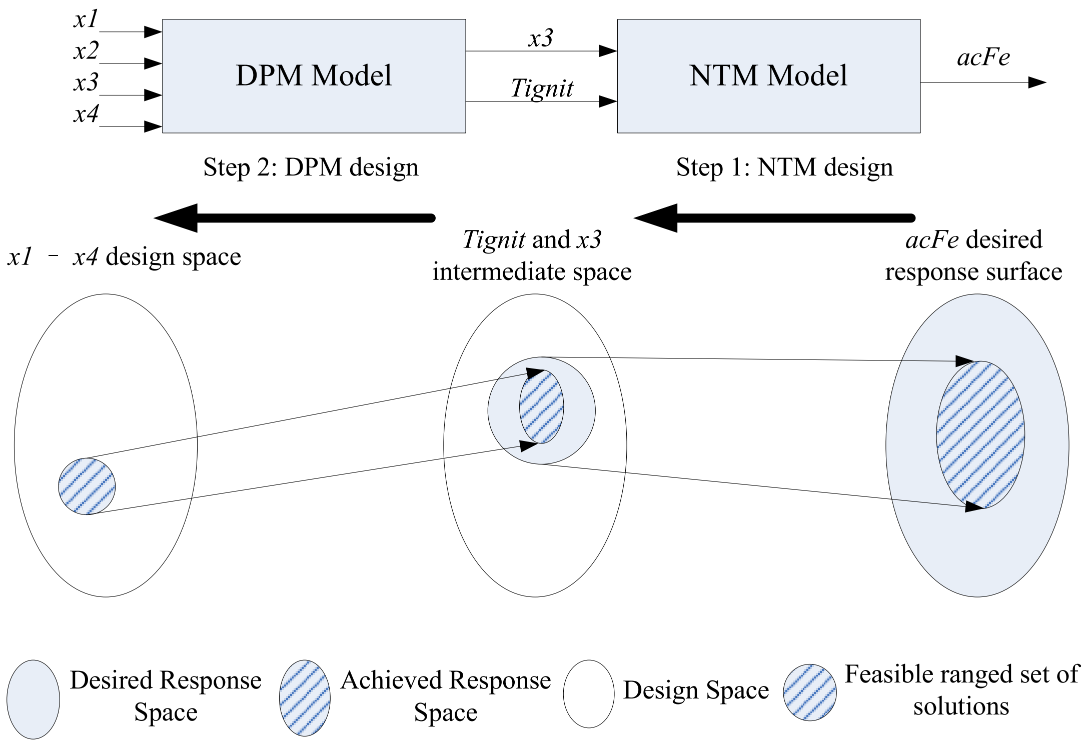


Figure 4. 10 - Inverse design exploration process of multiscale robust MESMs design

4.2.5 Robust Design Solution of MESMs Design Problem

For NTM model, the compromise DSP formulation is shown as the Table 4. 3. The design objective is to find out the feasible design range of Tignit and x3 which can make the performance acFe far from the response boundary, 5. The design freedom in this design problem can be defined according to designers' preference. In this design problem, design freedom in the volume fraction of voids is set as 0.02 and the critical temperature of chemical reaction as 0.2.

Table 4. 3 - cDSP formulation of NTM design

Given

Local regression model of NTM model: *f*;

Design freedom in the volume fraction of voids: $\Delta x3 = 0.02$

Design freedom in the critical temperature for chemical reaction initiation: $\Delta Tignit = 0.2$

y_0 mean response of NTM regression model;

Ymin Minimum response of NTM model with the variability of design variables (Response Boundary Exploration):

$$Y\min = y_0 - \left|\frac{\partial f}{\partial x_3}\right| \cdot \Delta x_3 - \left|\frac{\partial f}{\partial T_{ignit}}\right| \cdot \Delta T_{ignit}$$

Achieve $acFe \geq 5$ with consideration of uncertainty in NTM model

Lower Bound of response: $LRL \geq 5$

EMI_{target}=10

Find

Tignit: Critical temperature for chemical reaction initiation

x3: Volume fraction of voids

d_i^+, d_i^- deviation variables

Satisfy

Goals:

$$EMI \ / EMI_{\text{target}} + d_1^- - d_1^+ = 1$$
$$\text{where } EMI \ = \{[y_0 - LRL]/[-Y_{\min} + y_0]\}$$

Bounds:

$T_{ignit} = [1, 1.6](1000K)$; $x3 = [0.02, 0.1]$

Constraints:

$EMI_i > 0$

$$d_i^-, d_i^+ \geq 0$$

$$d_i^- \cdot d_i^+ = 0$$

Minimize

$$z_1 = d_1^+ + d_1^-$$

The computational codes for EMI calculation and deviation function are available in Appendix A.1 and A.2. Pattern search method in Matlab is used to find the mean values of design variable solutions ranges with minimum deviation function. The ranged set of solutions is obtained based on the mean values and the radius of design freedom. The solutions of the NTM design problem are shown in Table 4. 4. The minimum of the achieved response is 13.9, much larger than the desired response boundary. In addition, the *EMI* equals to 2.71, larger than one, which also means that the achieved response range is far from the desired response boundary. Therefore, this solution is acceptable.

Table 4. 4 - Robust Solution range of the NTM model

x3 range (mm)	*Tignit* range (1000K)	*acFe* achieved range	*EMI*
[0.06, 0.1]	[1, 1.4]	[13.9, 24.3]	2.71

After the design ranges of *x3* and *Tignit* are achieved, the intermediate design space is obtained. As shown in Figure 4. 11, the design range of *x3* becomes one of the design variable bound and the design range of *Tignit* becomes the design response requirements for the DPM model design.

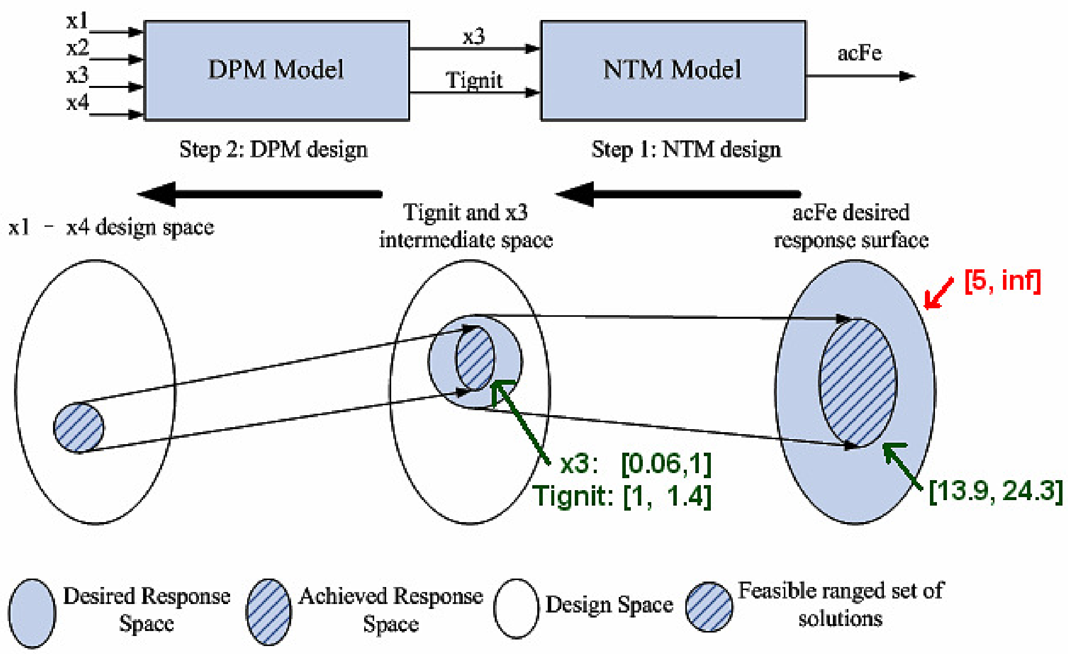


Figure 4. 11 - Intermediate design space of the NTM design

The compromise DSP of DPM design is shown in Table 4. 5. The design objective is to find out the feasible design ranges of *x1, x2, x3* and *x4* to achieve the performance within the design range of *Tignit*. However, the rough design exploration shows that the lower bound of the performance is always smaller than 1. It is impossible that the lower boundary of the performance can locate in the *Tignit* response range. In order to continue the design process, a new design constraint is set as the mean of the response should be larger than 1. In other words, although the lower boundary cannot locate in the feasible space of *Tignit*, the mean response should be larger than the minimal *Tignit*, and the upper boundary of the response should be smaller than the maximal *Tignit*. Since this problem provides the solutions of the whole design problem, the design freedom can be set as smaller than the previous step. The design freedom in the volume fraction of voids is defined as 0.01, which is much smaller than in previous step, because it is assumed that designers do not large design freedom in this step.

Table 4. 5 - cDSP formulation of DPM design problem

Given

Local regression model of DPM model: f;

upper 99% confidence interval: f_{upper};

lower 99% confidence interval: f_{lower};

Design freedom in mean radius of Al particles: $\Delta x1 = 0.0001$

Design freedom in the mean radius of Fe_2O_3 particles:

$\Delta x2 = 0.0001$;

Design freedom in the volume fraction of voids: $\Delta x3 = 0.01$;

Design freedom in the mean radius of voids: $\Delta x4 = 0.0001$;

y_0 mean response of NTM regression model;

Ymin Minimum response of lower 99% confidence interval DPM model with the variability of design variables (response boundary exploration):

$$Y\min = Min\left\{ y_{lower}(x) - \sum_{i=1}^{4} \left| \frac{\partial y_{lower}}{\partial x_i} \right| \cdot \Delta x_i \right\}$$

Ymax Maximum response of upper 95% confidence interval DPM model with the variability of design variables (response boundary exploration):

$$Y\max = Max\left\{ y_{upper}(x) + \sum_{i=1}^{4} \left| \frac{\partial y_{upper}}{\partial x_i} \right| \cdot \Delta x_i \right\}$$

Feasible range of *Tignit* identified in the NTM model;

Lower bound of response *LRL*: the minimum of *Tignit*, 1000K

Upper bound of response *URL*: the maximum of *Tignit*, 1400K;

EMI_{target}=10

Find

x1 : Mean of Al Particles

x2 : Mean of Fe_2O_3 Particles

x3 : Mean of Volume Fraction of Voids

x4 : Mean of Voids d_i^+, d_i^- deviation variables

Satisfy

Goals:

$$EMI \;/\; EMI_{\text{target}} + d_1^- - d_1^+ = 1$$

where $EMI_{upper} = \dfrac{Y\max - y_0}{URL - y_0}$,

$$EMI = Min\{EMI_{upper}\}$$

Bounds:

$$x1 = [0.0005, 0.0015];$$

$$x2 = [0.0002, 0.001];$$

$$x3 = [0.06, 0.1];$$

$$x4 = [0.0002, 0.001];$$

Constraint:

Mean of the performance should be larger than 1: $Y_{mean} > 1$

$$EMI_i > 0$$

$$d_i^-, d_i^+ \geq 0$$

$$d_i^- \cdot d_i^+ = 0$$

Minimize

$$z_1 = d_1^+ + d_1^-$$

The computational codes for EMI calculation and deviation function are available in Appendix A.3 and A.4. Pattern search method in Matlab is used to find the mean values of design variable solutions ranges with minimum deviation function. The ranged set of solutions is obtained based on the mean values and the radius of design freedom. The solutions of the DPM design problem are shown in Table 4. 5. The bound of *x3* is reduced in this design step and the feasible range of *x3* which can achieve desired responses is identified.

Table 4. 6 - Mean value of the robust solution of DPM

x1 range (mm)	*x2* range (mm)	*x3* range (mm)	*x4* range (mm)
[0.0005, 0.0007]	[0.0002, 0.0004]	[0.08, 0.1]	[0.00053, 0.00073]

The design response range of DPM model is shown in Table 4. 7. As expected, the lower boundary of the response is smaller than 1, but the mean of the response is exactly larger than the lower boundary of the response requirement, and the maximum of the response is also smaller than the upper boundary of the response requirement. Therefore, this solution is feasible according to the design requirements.

Table 4. 7 - Design response range from the robust solution of DPM model

Minimum of *Tignit* (1000K)	Mean of *Tignit* (1000K)	Maximum of *Tignit*(1000K)
0.7821	1.0001	1.3534

4.3 BENCHMARK DESIGN SOLUTION FROM IDEM

The design process of the IDEM method is the same as the design exploration method for adaptive design systems, because the propose method is modified from IDEM. Therefore, the first step of the design process is to find out the feasible design range in *Tignit* and *x3*. The solution is illustrated in Figure 4. 12.

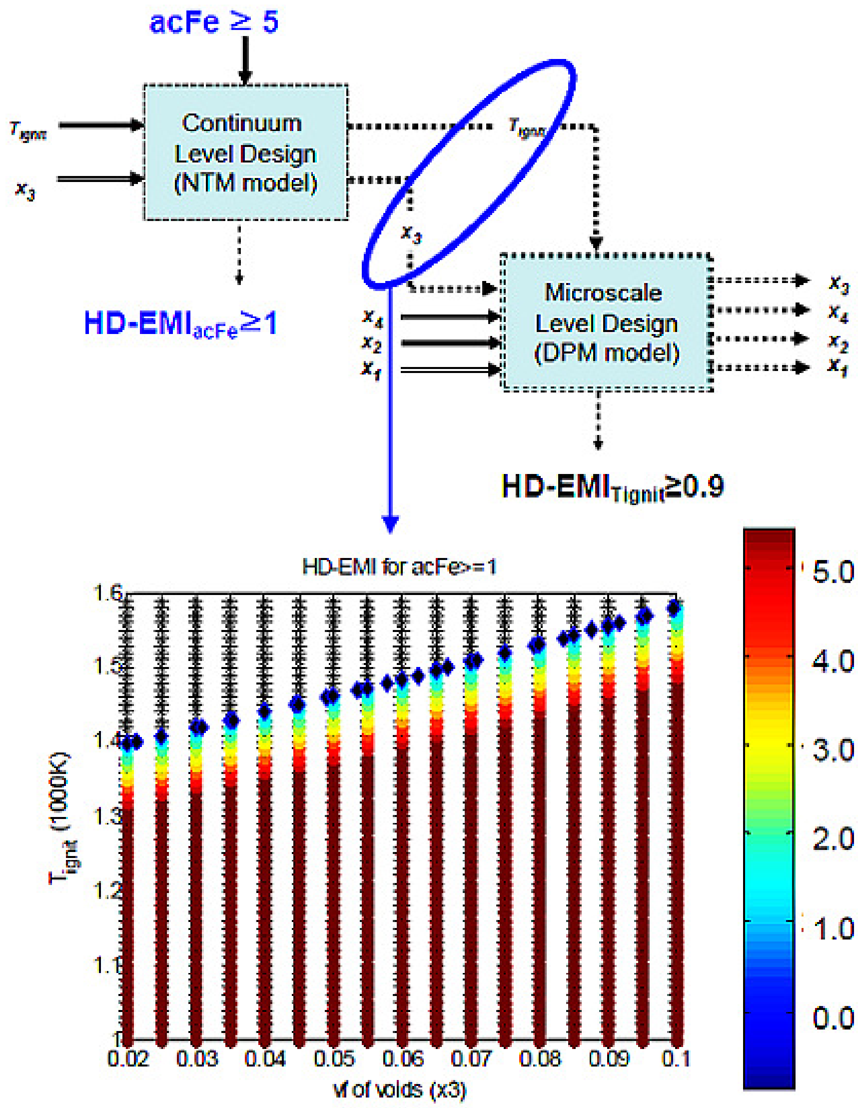


Figure 4. 12 - Obtained feasible range in *Tignit* and *x3* space [4]

As shown in Figure 4. 12, the boundary of the feasible space consisted by *Tignit* and *x3* is actually a function of *Tignit* and *x3*. In comparison to the feasible spaces of *Tignit* and *x3* obtained from the proposed method, the design space obtained from the IDEM is much larger, and the solution from the proposed method is actually a part of the space from IDEM.

Based on the obtained feasible space of *Tignit* and *x3*, the feasible design space of design variables (*x1~x4*) in DPM model can be identified. The discrete feasible points are illustrated as filled circles and the boundary points as void circles. The feasible discrete points and boundary points are illustrated in Figure 4. 13; the space is depicted at *x2*=0.0002(mm).

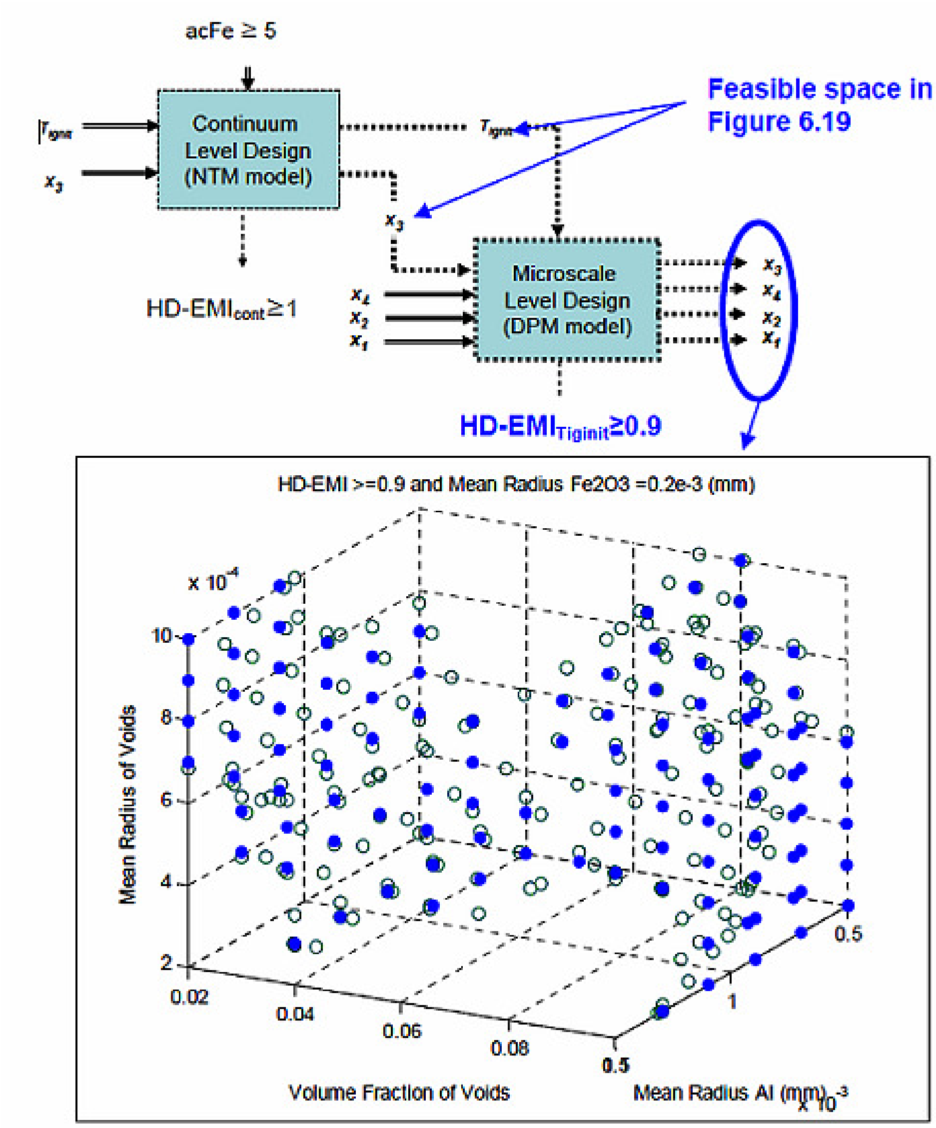


Figure 4. 13 - Feasible discrete points in *x1*, *x3*, and *x4* space (*x2*=0.0002mm) [4]

By increasing required minimum *HD-EMI*, the smaller feasible region is obtained. As shown in Figure 4. 14, the number of feasible points decreases as the required *HD-EMI* of *Tignit* increases, leaving only the more reliable (i.e., higher *HD-EMI*) design solution [4].

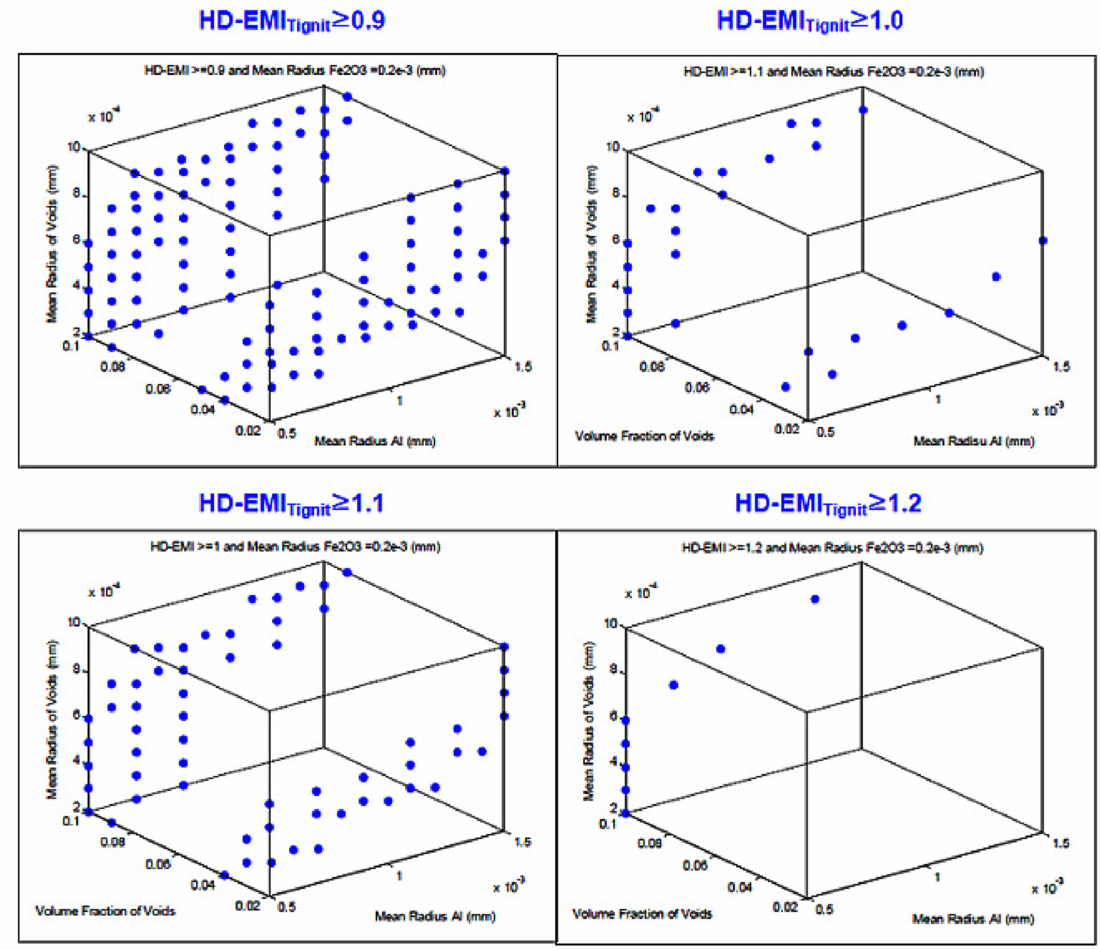


Figure 4. 14 - Reduced feasible region by increasing the required minimum *HD-EMI* for *Tignit* [4]

According to the IDEM, any solutions with *HD-EMI* larger than one are acceptable, and the higher *HD-EMI*s indicate better robustness against uncertainties in a model and variation in design variables [4]. In this design problem, higher *HD-EMI*s (i.e., larger than 1.2) are achieved when mean radius of Fe_2O_3 is 0.0002 (mm) and volume fraction of voids is 0.1, shown in Table 4. 8.

Table 4. 8 - Feasible discrete points at *HD-EMI* $_{acFe}$>1, *HD-EMI*$_{Tignit}$≥1.2

Mean Radius of Al (*x1*) (mm)	Mean Radius of Fe_2O_3 (*x2*)	Volume Fraction of Voids (*x3*)	Mean Radius of Voids (*x4*)	*HD-EMI*$_{Tignit}$
0.0005	0.0002	0.1	0.0002	1.23
0.0005	0.0002	0.1	0.0003	1.20
0.0005	0.0002	0.1	0.0004	1.20
0.0005	0.0002	0.1	0.0005	1.22
0.0005	**0.0002**	**0.1**	**0.0006**	**1.27**
0.0007	0.0002	0.1	0.0007	1.23
0.0009	0.0002	0.1	0.0008	1.24
0.0013	0.0002	0.1	0.0009	1.23

In Choi's dissertation, the solution with maximum *HD-EMI*$_{Tignit}$ (i.e., *HD-EMI*=1.27) is chosen as the most reliable solution. In the DEM-ADS, the mean of the ranged set of solutions is considered as the typical solution. A comparison of the design solution using IDEM and the DEM-ADS is shown in Table 4. 9. The solutions from two methods are very close. This is the same as what is expected, because the DEM-ADS uses the same basic idea as IDEM about the robust design. The only modifications are the solution search method and design freedom. The DEM-ADS is looking for a ranged set of solutions with largest *EMI*, while IDEM explores all feasible design space with specific *HD-EMI* larger than 1. Therefore, the solutions of the design exploration method for adaptive design systemss should be a subset of the IDEM solution. As shown in Table 4. 9, the mean of ranged set of solutions of the design exploration method for adaptive design systems is very close to the IDEM solution with the largest *HD-EMI*.

Table 4. 9 - A comparison of the design solutions using IDEM and DEM-ADS

Methods	*x1* (mm)	*x2* (mm)	*x3*	*x4*(mm)	*Tignit* (mean)	*acFe* (mean)
IDEM	0.0005	0.0002	0.1	0.0006	1002	21.17
DEM-ADS	0.0005	0.0002	0.1	0.000625	1001	20.638

4.4 VERIFICATION AND VALIDATION BASED ON SIMULATION-BASED MESMS DESIGN

The following section contains evidence for the verification and validation of the design exploration method for adaptive design systems presented in Chapter 3 by considering the design of the MESMs. First, the validity of the design solution is examined. Then, the results obtained from completing the MESMs example problem are discussed in terms of validating the proposed method to the systems robust design.

One of the main goals in completing the MESMs example problem is to provide evidence in the verification and validation of the proposed design exploration method for adaptive design systems for robust design of systems. In the following sections, ways of completing the MESMs example problem adds value to the domain-specific structural validity and domain-specific performance validity of the proposed method are presented.

4.4.1 Domain-Specific Structural Validity

Domain-specific structural validity relates to the appropriateness of the selected example problem and designers should answer the question, “Is the example problem used in demonstrating the method an appropriate choice?” It is asserted that the MESMs example problem is an appropriate choice for testing the effectiveness of the proposed design exploration method for adaptive design systems in improving efficiency of solution search process because of the following characteristics of the design problem:

Well Defined Design Problem

This design example was used by Hae-jin Choi in his dissertation [4] as an example to validate the IDEM. Therefore, this design problem contains a clearly defined problem statement with specific design variables, bounds, constraints, goals and preferences. Each of the descriptions is necessary for the successful implementation of the design exploration method for adaptive design systems. In addition, due to previous knowledge of the design problem, sufficient design information is available, so that it is not necessary to discrete explore the whole design process. Although this design problem is not exactly adaptive design, it shares the same characteristic: sufficient design information is available. Furthermore, the system structure and subsystem model information with uncertainty analysis is known or easily determined for the MESMs design problem.

MESMs Design has a multi-level coupling

The MESMs design includes two different levels, the continuum level and microscale level, each of which includes a complex subsystem simulation model. This design problem is a typical complex system with multi-level coupling. Therefore, due to the complex system nature of the MESMs example problem, it is an appropriate choice for applying the proposed DEM-ADS presented in Chapter 3.

Due to these two features, it is shown that the MESMs design problem is an appropriate design example to validate the advantage of DEM-ADS in improving the efficiency of the solution search process in a system design.

4.4.2 Domain-Specific Performance Validity

Domain-specific performance validity relates to the outcome of applying the method to an example problem and is used to ask the question, “Does the application of the method to the example problem produce useful results?" To adequately address this question, two topics are considered: the usefulness of the numerical design solution and the overall usefulness of the design exploration method for adaptive design systems.

Appropriateness of the MESMs Design Solutions

The results obtained from the MESMs design problem by the design exploration method for adaptive design systems are reasonable. The solutions are very close to those from IDEM. Since the solutions from IDEM have been demonstrated by Hae-Jin Choi in his PhD dissertation [4], the solutions in this thesis are also acceptable.

Convergence of the Solution Search

The MESMs example is solved using pattern search in this thesis. Therefore, it is important to determine whether the optimization algorithm stops at the optimal point or stop because it reaches the maximum number of iterations. The convergence plots of each solution search process are checked as shown in Figure 4. 15 and Figure 4. 16.

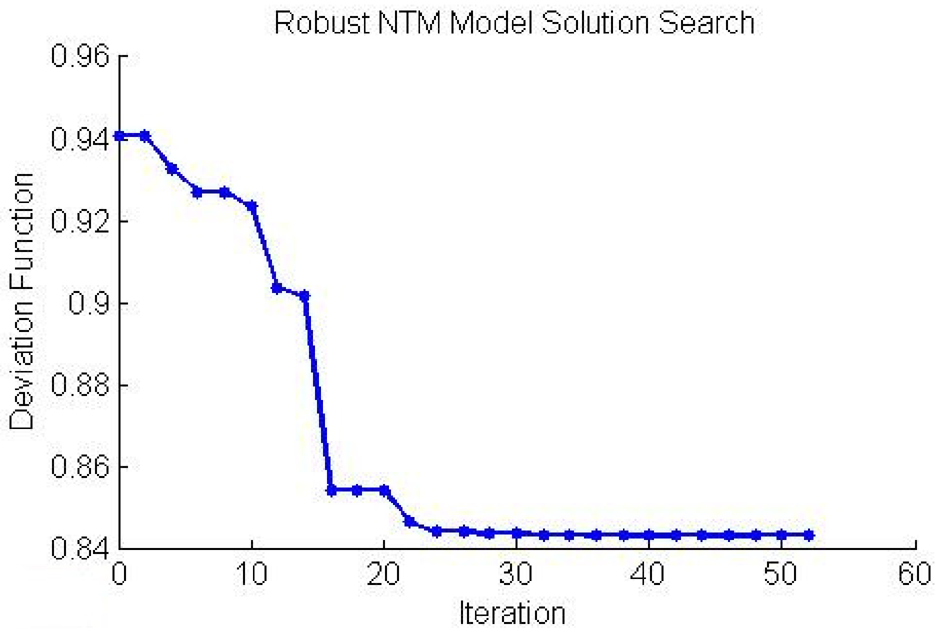


Figure 4. 15 - Convergence plot of robust NTM model solution search

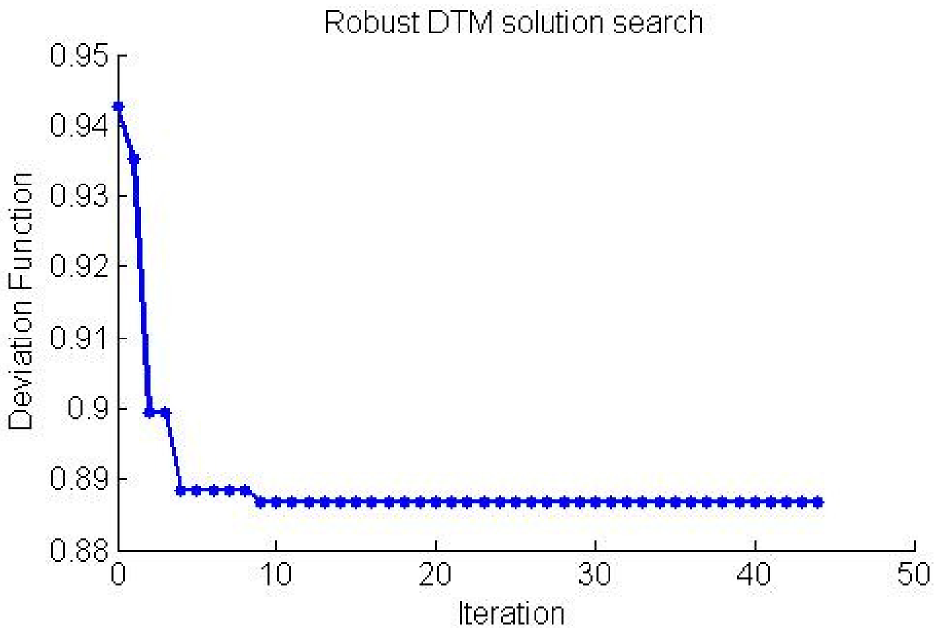


Figure 4. 16 - Convergence plot of robust DPM solution search

Both the convergence plots show that the solution search processes converge. The optimization processes stopped because the optimum criteria have been achieved. Therefore, these results from the optimization routine are acceptable.

Starting Point Analysis for the MESMs Design

The internal consistency of the MESMs design solution is also tested with starting point analysis. The MESMs design problem is solved using an optimization routine (pattern search method). Therefore, it is important to determine if the selected starting point in each solution search results in a robust, stable solution that most closely meets design goals. A starting point analysis that implements ten different starting points is completed for each solution search. The starting points are at 10% increments of the design variable bounds. The deviation function value is measured at each starting point. The starting point analysis of robust NTM model is shown in Figure 4. 17. The solution is robust to changes in starting point, and the best solution of NTM model is identified.

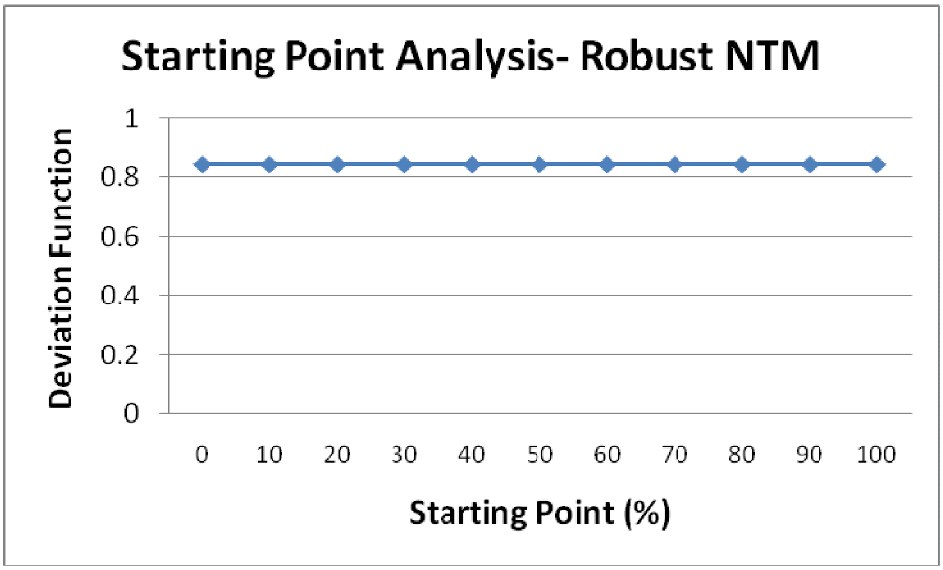


Figure 4. 17 - Starting point analysis of robust NTM solution search

The robust DPM solution search shows high percentage of local (not global) minimum results. The constraint (i.e., the mean of response should be larger than 1 or EMI equals to -1) in DPM solution search makes the design problem highly nonlinear. Also, the number of design variables increases the probability that implementing the optimization routine will result in the local minimum. Therefore, a slightly different approach is taken in order to ensure a reasonable solution is reached. The starting points of DPM solution search are chosen as points close to the IDEM solutions, since the IDEM solutions are already known. The response is robust to the changes near the expected solution. And, different starting points which are far from the expected solution are implemented and the results show that all of the deviation function values obtained are larger than that obtained from the points near the expected solution. Therefore, the current solution can be considered as reasonable.

Usefulness of the design exploration method for adaptive design systems in the MESMs Design

Since the evidence supports the validity of the MESMs design solution, it is important to identify whether the design exploration method for adaptive design systems is useful in the MESMs design. Simply obtaining valid solution from implementing the proposed method is not sufficient for its domain-specific performance validity. The benefits experienced from implementing the proposed method in the MESMs design should also be investigated.

The usefulness of applying the design exploration method for adaptive design systems to the MESMs example problem is demonstrated in decreased computational cost while keeping the accurate of solutions. Efficient solution search method, such as pattern search method, is implemented in the DEM-ADS. Compared to the exhaustive search method used in IDEM, the number of function calls of the DEM-ADS is reduced and total evaluation time is also shorter than IDEM. The comparison of the computational cost for IDEM and the DEM-ADS is shown in Table 4. 10. The number of evaluation function calls can represent the computational cost for two methods. The number of calls information of IDEM is obtained from [13]. The comparisons indicate that the DEM-ADS requires fewer evaluation function calls, which means that the solution search process of the DEM-ADS is more efficient than the IDEM.

Table 4. 10 - Comparison of the computational cost for IDEM and the design exploration method for adaptive design systems

Design Methods	IDEM		Design exploration method for adaptive design systems	
Simulation Models	NTM model	DPM model	NTM model	DPM model
Number of calls	909	4374	101	162

The solution from the design exploration method for adaptive design systems is very close to the solution of IDEM. Therefore, the accuracy of the solutions is not compromised to the efficient solution search method, although the design freedom is reduced in the proposed method. However, there is no evidence that the reduced design freedom would influence the performance or future design. In addition, the inverse design exploration process guarantees the robustness of solutions against model uncertainty and slight variable deviations. Therefore, the solutions obtained in the design exploration method for adaptive design systems are robust.

Limitations of Design Freedom Defined in Each Design Step

In IDEM, the design freedom, number of feasible solutions, is determined by the results of EMI evaluations of all discrete points in each design step. Therefore, designers do not need to worry about the size of design freedom. As long as there are some solutions existing, a set of solutions can be obtained. In DEM-ADS, the design freedom is defined by designers in the beginning of each design step. Therefore, it is important to determine how large the design freedom is appropriate for the design step. However, sometimes, it may be difficult for designers to make such decisions, because there may be no solutions if design freedom is too large.

For instance, different size of design freedom of DPM model in DEM-ADS design problem is examined. When the size of design freedom is defined smaller, as shown in Table 4. 11, the solution is close to the original solution shown in Table 4. 6. The solution with smaller design freedom of DPM model in DEM-ADS is shown in Table 4. 12, which is actually a subset of solutions with the original solution. If the size of design freedom continues to reduce, designers can always obtain specific solutions with smaller ranged set. However, the designers have a smaller solution pool to choose appropriate solutions in order to deal with uncertainties in the system.

Table 4. 11 - Smaller design freedom of DPM model in DEM-ADS

x1	*x2*	*x3*	*x4*
0.0001	0.0001	0.01	0.0001

Table 4. 12 - Set of solutions of DPM model with smaller design freedom in DEM-ADS

x1 range (mm)	*x2* range (mm)	*x3* range (mm)	*x4* range (mm)
[0.0005, 0.0006]	[0.0002, 0.0003]	[0.09, 0.1]	[0.00058, 0.00068]

When the size of design freedom become larger, such as the design freedom shown in Table 4. 13, there may be no solutions existing. Due to the strict design constraints and bounds in the design problem, there are no feasible solutions exiting when design freedom is defined as Table 4. 13. Obviously, if design freedom continues becoming larger, no feasible solutions will exist. Therefore, it is important for designers to make decisions about the appropriate size of design freedom, and it is possible that designers may have to try different sizes of design freedom in order to obtain a set of solutions with satisfactory EMI.

Table 4. 13 - Smaller design freedom of DPM model in DEM-ADS

x1	*x2*	*x3*	*x4*
0.0004	0.0004	0.04	0.0004

Therefore, in some design problems, it is difficult for designers to make decisions about the size of design freedom in each design steps. It may depend on designers' expertise to make correct decisions. In some cases, designers may have to try different sizes of design freedom before feasible solutions obtained. This is one limitation of DEM-ADS.

To summarize, the design exploration method for adaptive design systems to the MESMs design is a valuable design strategy because the computational cost was decreased. A visual representation of the value added to the verification and validation of the developed design exploration method for adaptive design systems provided in Chapter 4 is shown in Figure 4. 18.

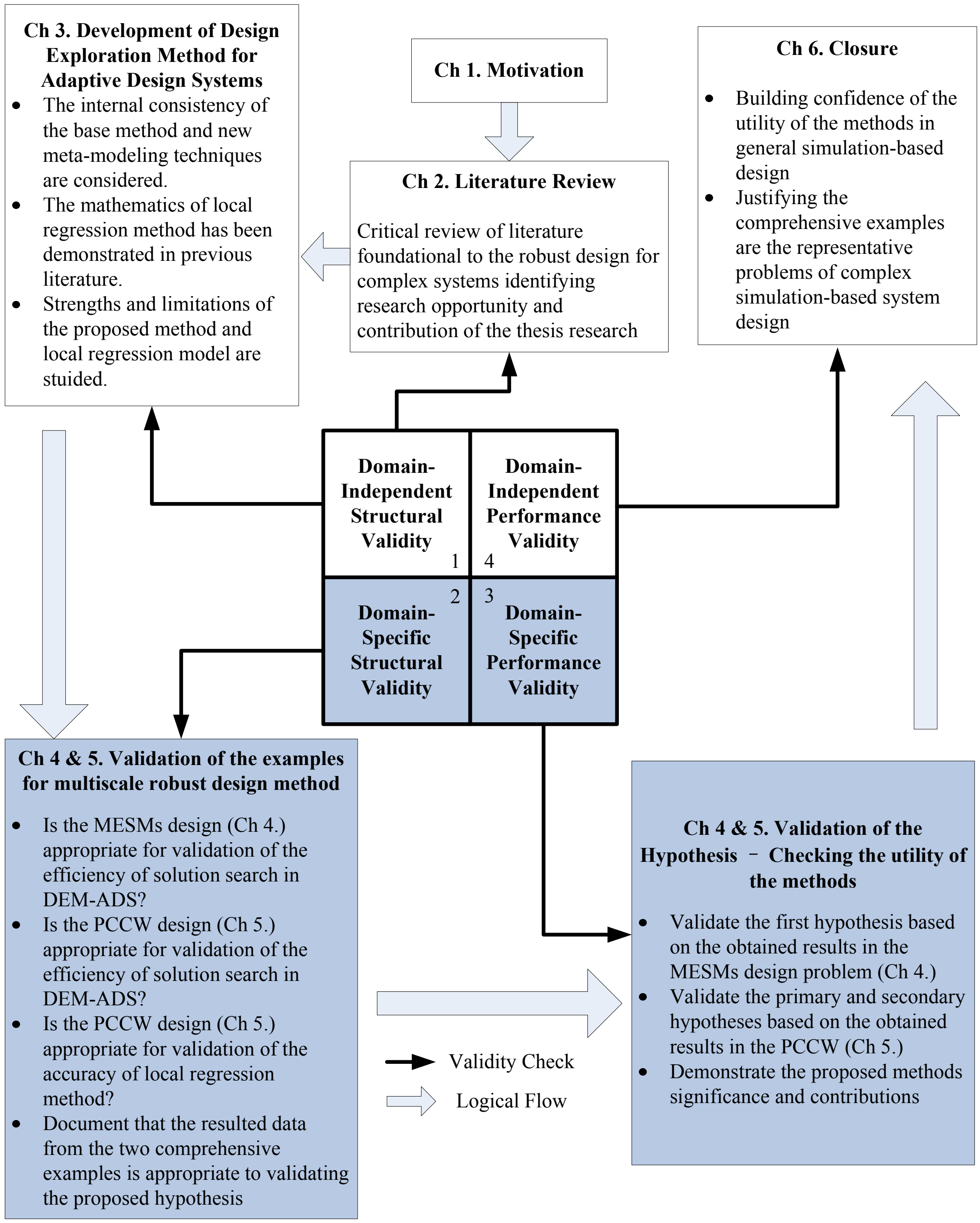


Figure 4. 18 - Value added to verification and validation of the DEM-ADS – Chapter 4

4.5 SYNOPSIS OF CHAPTER 4

The completion of the MESMs design problem adds value to the validation of the design exploration method for adaptive design systems in improving the efficiency of solution search in systems design, which is the primary hypothesis in this thesis. The MESMs design problem is a typical system design problem with a multi-level coupling and the uncertainty management is necessary, so that this design problem is an appropriate design example for adaptive design systems. Because this design problem does not require the discrete design exploration due to sufficient design information, IDEM may be too expensive to solve this design problem. In the results of this design problem, it is also shown that DEM-ADS can provide designers with similar accurate solutions, while the efficiency of solution search of DEM-ADS is much better than IDEM according to the comparisons of the number of function calls. Therefore, the MESMs design problem in Chapter 4 addresses the Domain-dependent Structural Validity and Domain-dependent Performance Validity of the primary hypothesis, the improved efficiency of solution search of DEM-ADS.

In next chapter, Chapter 5, the PCCW design problem is introduced to validate both primary and secondary hypotheses. In the PCCW design problem, the design problem is not only appropriate to validate the efficiency of solution search in DEM-ADS, but also appropriate to validate the accuracy of the surrogate model. In addition, the PCCW design problem is not classified to material design. Therefore, in Chapter 5, it is also shown that the DEM-ADS can also be implemented in design problems beyond the material design domain. The completion of Chapter 5 brings contributions to the completion of Domain-dependent Structural Validity and Domain-dependent Performance Validity of both primary hypothesis and secondary hypothesis.

CHAPTER 5
SIMULATION-BASED PHOTONIC CRYSTAL COUPLER AND WAVEGUIDE DESIGN PROBLEM

In this chapter, the primary and secondary hypotheses are both validated. In the primary hypothesis, the design exploration method for adaptive design systems (DEM-ADS) is proposed to efficiently to find ranged set solutions against uncertainty in the system. In the secondary hypothesis, the local regression model is proposed to improve the accuracy of the meta-model for a highly nonlinear model. In this chapter, a comprehensive example, the simulation-based Photonic Crystal Coupler and Waveguide (PCCW) design example, is employed to show the better efficiency of solution search in DEM-ADS and more accurate surrogate modeling by local regression method. The PCCW simulation and analysis models are logically connected and used for predicting the final performance of the PCCW. The results of this design example bring contributions to the completion of Domain-dependent Structural Validity and Domain-dependent Performance Validity of both primary hypothesis and secondary hypothesis.

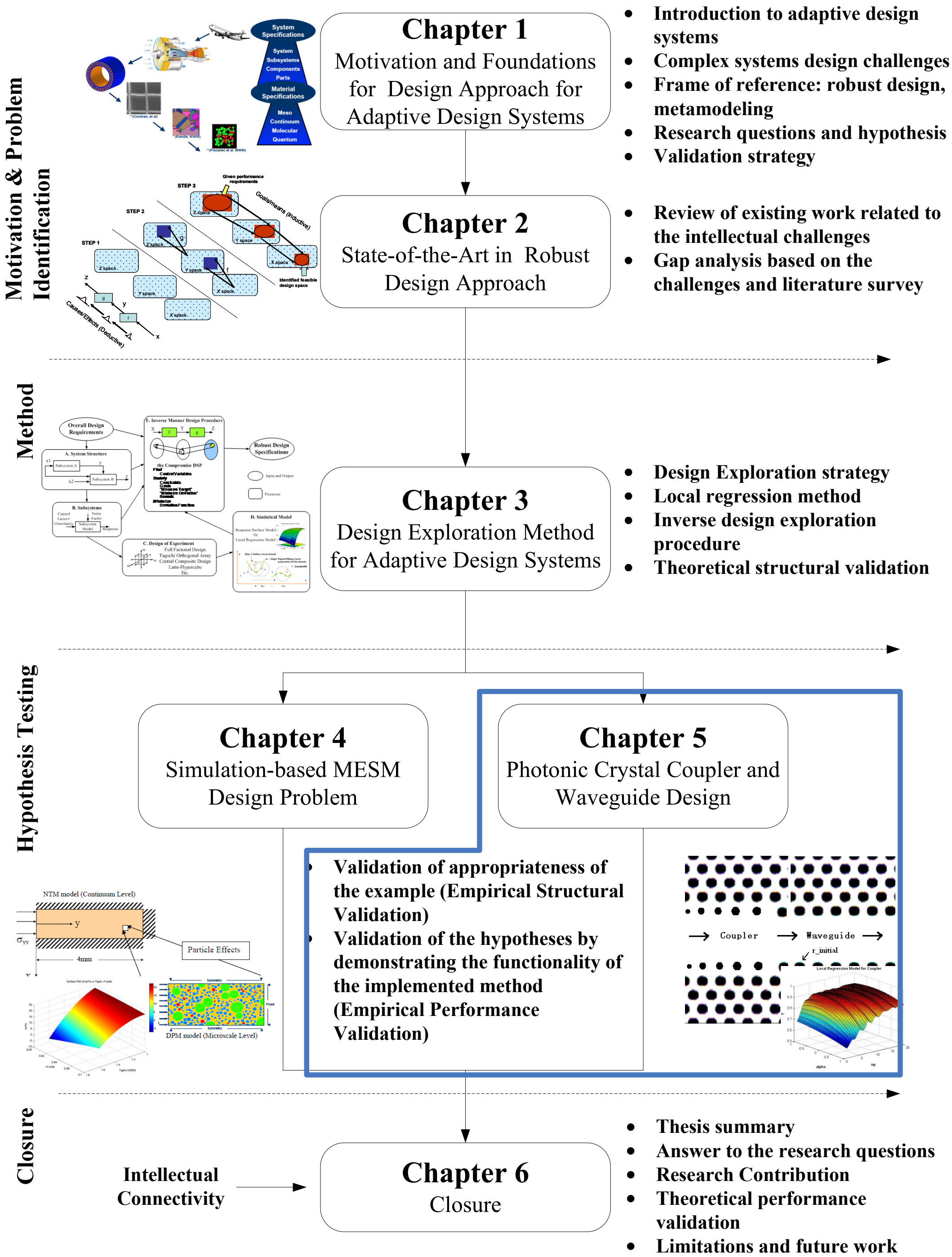


Figure 5. 1 - Thesis roadmap

In Section 5.1, the photonic crystal coupler and waveguide model are introduced. The two models are logically interfaced and formulate a simulation model chain. The value of completing this design problem is also addressed and the design example is validated as an appropriate example for demonstrating the utility of the DEM-ADS and the local regression method. In Section 5.2, the DEM-ADS is implemented to solve this design problem in detail and the local regression method is used to fit the highly nonlinear coupler model. The accuracy comparisons of local regression model and response surface model show the advantage of local regression method in fitting nonlinear data. In Section 5.3, the non-robust solution is explored to compare with the robust solution. In Section 5.4, the IDEM solution is explored and compared to the DEM-ADS solution. The comparisons show the advantages of the DEM-ADS. In Section 5.5, the solutions and hypotheses are validated by checking whether the DEM-ADS and local regression are useful for the complex PCCW robust design problem.

5.1 INTRODUCTION OF SIMULATION-BASED PHOTONIC CRYSTAL COUPLER AND WAVEGUIDE (PCCW) DESIGN

In Section 5.1, an overview of the simulation-based photonic crystal coupler and waveguide design problem is presented. The design problem is completed with the help of Dr. Vivek Krishnamurthy and Dr. Benjamin Klein from Electrical and Computer Engineering Department at Georgia Tech Savannah.

5.1.1 Overview of the Simulation-based PCCW Design Problem

Slow light waveguides provide superior optical processing capability because they enhance light-material interaction. Direct coupling of light from a conventional waveguide to a slow light waveguide usually is known to result in a large impedance mismatch [51, 52]. A coupler is required to match efficiently the impedance between a conventional waveguide and periodic waveguide. The most important purpose of the coupler is to make sure that the light enters the coupler at the linear dispersion regime, and as the light propagates, the linear dispersion regime adiabatically transforms into flat dispersion regimes at the periodic waveguide end [53]. The adiabatic variation [51, 52, 54] of the dispersion properties of light in the coupler can either be linear or non-linear.

The simulation presented in this example is carried out using a 2D planewave-based modal method. In this approach, the device is sliced into layers along the propagation (z) direction. Each layer is uniform along the z direction. Using the planewave expansion technique, the propagating and evanescent modes of each layer are obtained numerically, assuming a periodic supercell in the direction perpendicular to the direction of propagation (x). Following this, a scattering matrix method is used to match modes at the interfaces between the layers, and obtain the reflection and transmission. The simulation domain in each case is terminated with a semi-infinite slow-light waveguide, which is achieved numerically by projecting the fields onto the basis set of outgoing Bloch waves. This is done to avoid resonances associated with the finite length of the slow-light waveguide. We have tested the boundary condition to verify that adding additional layers to the semi-infinite slow-light waveguide does not affect the transmission [55].

In photonic crystals, it is well known that the periodically etched holes in photonic crystal waveguides can be designed to obtain slow light. The photonic crystal considered is a high refractive index medium with air holes in it as shown in Figure 5. 2. An effective index of the medium is considered to be 2.811 to reduce the problem from 3D to 2D [55]. The black circles in Figure 5. 2 are the air holes. The radius of the end air hole in the coupler equals to that of the initial air hole in the waveguide. The radius of air holes in the coupler gradually increases from the left side to the right side of the coupler [55].

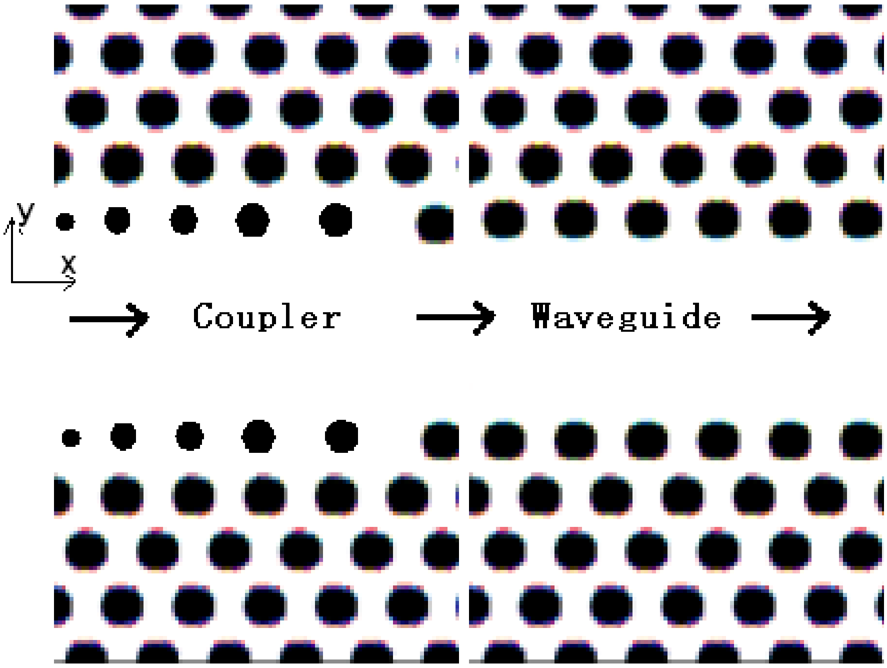


Figure 5. 2 - Photonic crystal coupler and waveguide structure[55]

A defect etched in the crystal gives rise to odd and even band gap guided modes. Photonic crystals can be designed such that within the band gap region, just a single mode exists. Figure 5. 3 gives the dispersion relation of the waveguide. Note that at the band edge, the dispersion relation becomes flat indicating the slow light region. The transmission spectrum from a slab waveguide to the photonic crystal waveguide without using a coupler is shown in Figure 5. 4. A normalized frequency, 0.2663 is considered to be the slow light frequency.

Further detail information about the simulation-based PCCW design can be found in [55].

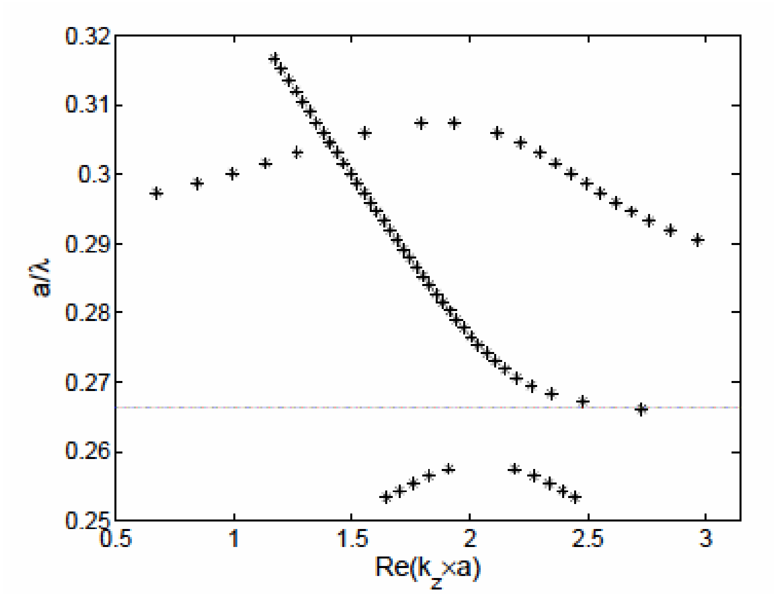


Figure 5. 3 - Dispersion diagram of the photonic crystal waveguide with periodicity, a, radius of air holes, r=0.3a for TM polarization [55]

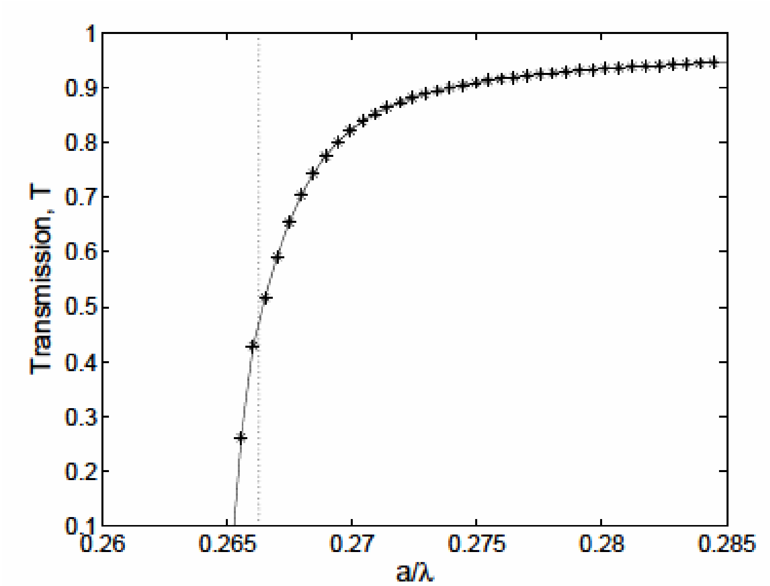


Figure 5. 4 - Transmission at the conventional waveguide - photonic crystal waveguide interface [55]

5.1.2 System Design Analysis of the Simulation-based PCCW Design Problem

The coupler model and waveguide model are working together to obtain a good transmission response. The interface of two models is the radius of air hole in the right end of the coupler model and the radius of the air holes in the waveguide model. The value of the radius of these air holes is equivalent shown as Figure 5. 5.

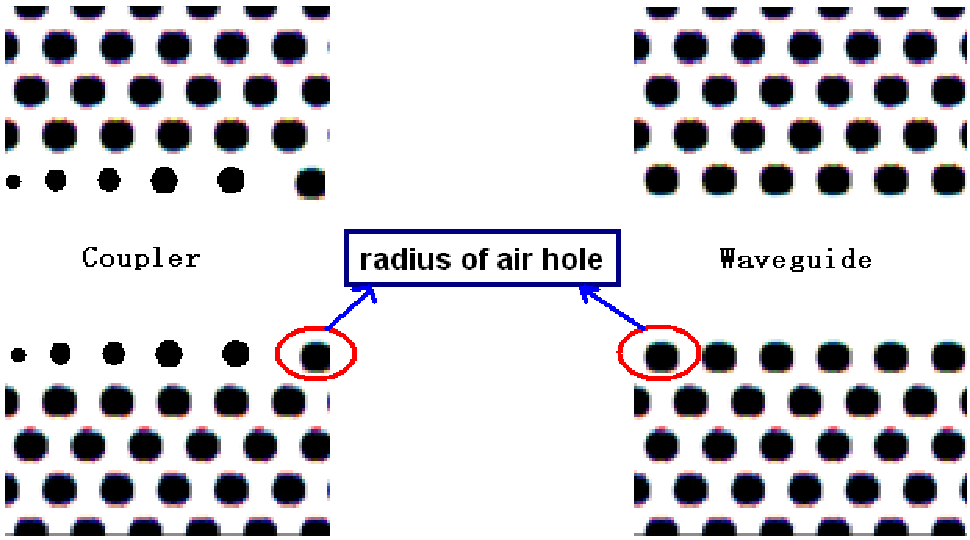


Figure 5. 5 - Connecting the coupler model and waveguide model

This design problem is a typical system design problem on the same design scale, which includes two subsystems connecting to each other.

5.1.3 Value in Completing the Simulation-based PCCW Design

Addressing Research Questions

The simulation-based photonic crystal coupler and waveguide design is selected because of its similarity to the topics discussed in the research questions. The simulation-based PCCW design is a clearly defined system design problem and it is also adapted from a photonic crystal design problem consisting of the same simulation models [55]. Therefore, it is an adaptive design systems problem and design information is sufficient so that it is not necessary to explore discretely the whole design space. In addition, this design problem is a typical system design problem including a shared design variable by two models. The two models can be decoupled from the system and explored in parallel or in sequence. In this problem, the two models are analyzed in sequence to find solutions. Therefore, the successful completion of the DEM-ADS to the PCCW design problem addresses the usefulness of uncertainty management in a system design problem (primary research question). The other motivation for this design problem is to demonstrate the usefulness of the local regression method to fit the nonlinear model (secondary research question). The coupler model is a nonlinear model, and it may be difficult for a low-order response surface model to create an accurate surrogate model. The local regression method may be an alternative statistical method to be used in this design problem. Therefore, the PCCW design problem is appropriate to validate both of the hypotheses in this thesis.

Verification and Validation of the DEM-ADS and Local Regression Method

In terms of validating the DEM-ADS and local regression method, the PCCW example problem is useful in demonstrating the domain-specific structural validity and domain-specific performance validity of the proposed approaches. The PCCW example problem is also intended to illustrate the key advantages of the DEM-ADS, which can efficiently find a ranged set of solutions against uncertainty propagation, and present the advantage of the local regression method, which can reduce the uncertainty in single model caused by inaccurate surrogate model.

5.2 PCCW ROBUST DESIGN PROCESS AND SOLUTION

In the following section, the design of the PCCW is presented. The design process is introduced by step by step of the DEM-ADS in details. In Section 5.2.1, the design task clarification and system structure of the PCCW design is studied. In Section 5.2.2, the uncertainty of each subsystem is analyzed. In Section 5.2.3, design of experiment and local regression model are implemented to create surrogate models. In Section 5.2.4, the inverse design exploration process is employed to find a raged set of solutions robust to the uncertainty in the model chain. The successful implementation of the DEM-ADS in the design of the PCCW builds confidence in the validation of the DEM-ADS.

5.2.1 Design Requirements and System Structure of the PCCW Design

In system design view, the waveguide system includes two parts, waveguide model and coupler system. The design variable *rh* is shared by two models. The system has two objectives, maximizing both transmission of waveguide and coupler. *cr* in this problem is the change rate of the holes, and *np* is the number of periods in the coupler. There are two objectives in this design problem: transmission of waveguide, called as $T_{waveguide}$, and transmission of system, called as T_{system}. The goal of this design problem is to maximize the objectives. The system design problem is shown in the Figure 5. 6.

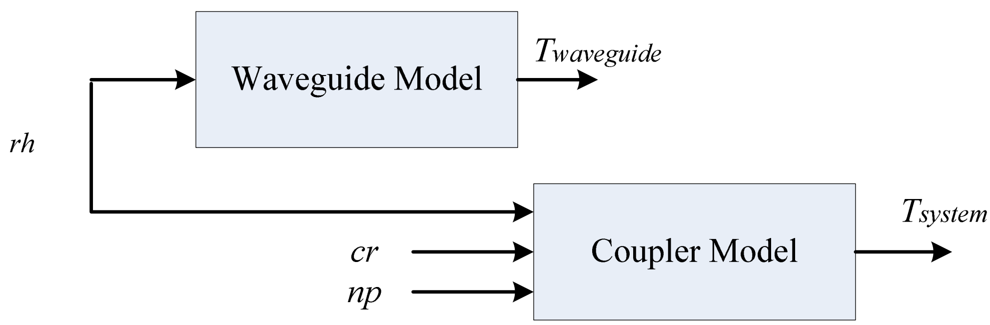


Figure 5. 6 - System design problem flowchart

5.2.2 Subsystem Analysis of PCCW Design

Since photonic crystal design is complex and hierarchical, it is unreasonable to assume the system model is deterministic – there are no random errors in a system response. In addition, uncertainty is associated with model-based prediction for some reasons. Different kinds of uncertainty exist in two models.

Coupler Model Analysis

In the coupler model, one important uncertainty comes from the fabrication of the photonic crystal, which is as important as intrinsic losses in the design of nano-scale devices [55]. Another uncertainty existing in the model is "model parameter uncertainty", which is due to a combination of limited data and nonparametric system noise. This is the typical type of uncertainty that employs computationally intensive models. The coupler simulation model is the model with high computationally cost, so that it is necessary to implement meta-modeling technique to reduce the cost. According to the rough design space exploration, the model shows a highly nonlinear feature. Therefore, the regression model may also include the uncertainty due to the poor fits.

Waveguide Model Analysis

Fabrication error is also an uncertainty in the waveguide model. In this model, the size of air holes is assumed as constant along the length of waveguide model, but that is almost impossible to happen due to fabrication errors. In addition, the original waveguide model is also computationally intensive. Thus, it is necessary to create a surrogate waveguide model in order to keep the computational cost within a feasible range. The accuracy of the surrogate waveguide model also influences the model uncertainty. Therefore, the model uncertainty is assumed as an important uncertainty in the waveguide design problem.

5.2.3 Design of Experiments and Model Regression

In this work, Phoenix Integration ModelCenter® is used for design of experiment of coupler model and waveguide model. In order to create an accurate model, the Latin-Hypercube Sampling is set as 100 levels for coupler model and 20 levels for waveguide model, shown as Figure 5. 7.

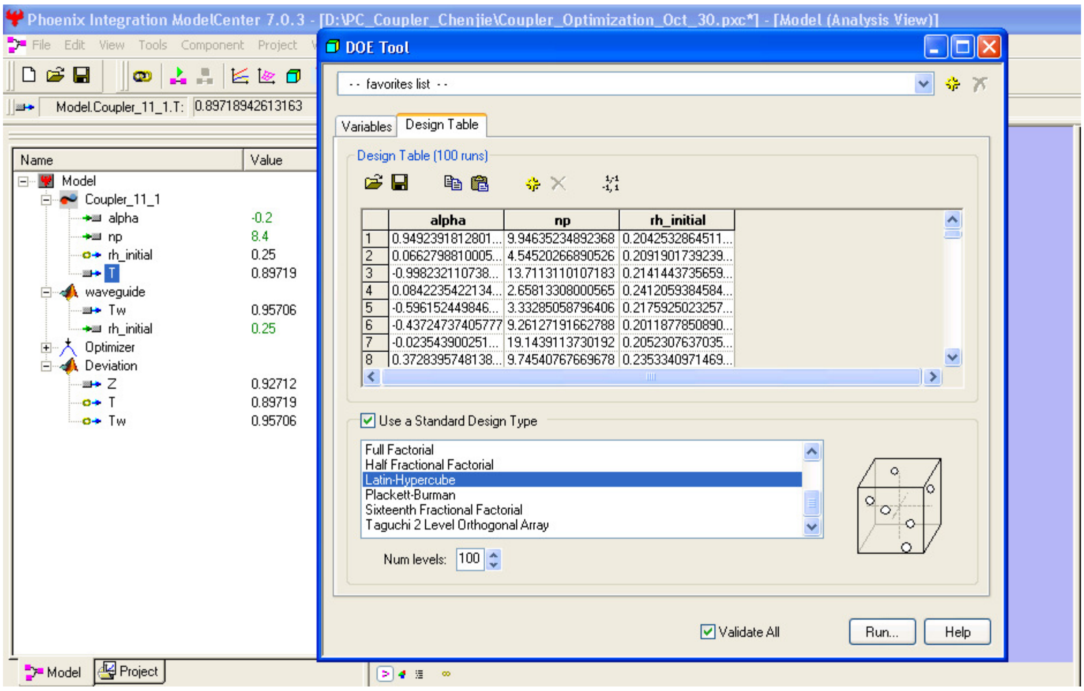


Figure 5. 7 - Design of Experiments in ModelCenter

The response surface model for coupler model is fit to the data obtained from the Design of Experiments using ordinary least squares regression techniques and the software package ModelCenter. A full cubic response surface model is chosen and the regression function is shown as follows:

$$
\begin{aligned}
T = & -3.716 + 0.905\cdot x_1 - 0.00189\cdot x_2 + 55.528\cdot x_3 - 0.0545\cdot x_1^2 - 0.00422\cdot x_2^2 - 232.156\cdot x_3^2 \\
& + 0.000276\cdot x_1\cdot x_2 - 7.813\cdot x_1\cdot x_3 + 0.498\cdot x_2\cdot x_3 - 0.0253\cdot x_1^3 + 0.000121\cdot x_2^3 + 315.739\cdot x_3^3 \\
& + 0.000787\cdot x_1^2\cdot x_2 - 0.0652\cdot x_1^2\cdot x_3 + 0.000225\cdot x_1\cdot x_2^2 - 0.00558\cdot x_1\cdot x_2\cdot x_3 + 15.766\cdot x_1\cdot x_3^2 \\
& - 0.00354\cdot x_2^2\cdot x_3 - 0.843\cdot x_2\cdot x_3^2
\end{aligned}
\tag{5.1}
$$

where *cr* is *x1*, *np* is *x2* and *rh* is *x3*, the following equation can be obtained as the regression function. The R-square value of this response surface model is 95.13%.

"LOCFIT" is used to create local regression model, which is a software system written by Clive Loader [48, 56], for fitting curves and surfaces to data, using the local regression and likelihood methods.

The GCV is computed for local quadratic fits to the coupler model data and a range of smoothing parameters: $0.2 \le \alpha \le 0.7$. The result is shown in Figure 5. 8 as a cross validation plot. The plot uses the fitted degrees of freedom as the horizontal axis and the GCV as the vertical axis. The smoothing parameter is $\alpha = 0.7$ on the left, decreasing in steps of 0.05 to $\alpha = 0.2$ on the right. The first few points, with fewer degrees of freedom, and the last one with largest degree of freedom, produce relatively large GCV scores in the GCV plot, indicating these fits are inadequate. Small degree of freedom also represents a smooth model with very little flexibility. The last few points, with larger degree of freedom, produce a small GCV score, which however represents a noisy model showing too many features. The points, in the middle of the plot with the degree of freedom from 20 to 24, have similar GCV, which means there is little to choose between the fits. However, the point with $\alpha = 0.35$ has the largest degree of freedom among these points. This smooth parameter should be chosen in order to have a good fit. Since the GCV plot is just one way to choose bandwidth/smooth parameter in local regression, it is not necessary to compare other α around 0.35. Therefore, for this coupler model, the smooth parameter is chosen as 0.35, quadratic local polynomial is employed, and tri-cube weight function is used. The smoothing parameter from 0.3 to 0.4 can create similar accurate models according to the residuals plots. In this thesis, the smoothing parameter is set as 0.35.

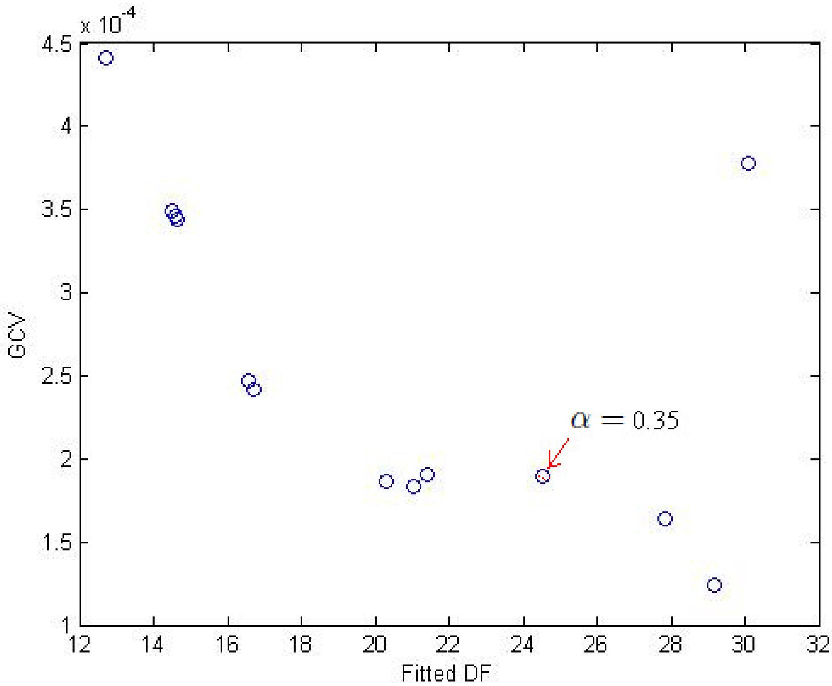


Figure 5. 8 - Cross validation plot for the coupler model data

Error Analysis of Response Surface Model and Local Regression Model

The accuracy of the response surface model and the local regression model is examined using 20 randomly selected validation points from the DOE data set. Error is defined as the difference between the actual response from the simulation analysis, y, and the predicted value, $\hat{y}$, from either the response surface model or the local regression model. The maximum absolute percent error, the average absolute percent error, and the RMSE for the 20 validation points are summarized in Table 5. 1.

As seen in Table 5. 1, the local regression model has lower maximum absolute error, lower average absolute error and lower RMSE values for the response than the response surface model. It is not surprising that the local regression model is much better than the full cubic response surface model which has a fair R-square value (only 95%). In summary, it appears that both models predict the response well, but the local regression model has an obvious advantage in overall accuracy because of lower average error and root MSE value.

Table 5. 1 - Error Analysis of Response Surface and Local Regression Model

Third order response surface	
Max (% error)	5.36
Avg (% error)	1.71
RMSE, %	2.18
Local Regression	
Max (% error)	1.70
Avg (% error)	0.786
RMSE, %	0.945

The residual plots of the local regression model and response surface model are shown in Figure 5. 9 and Figure 5. 10. The maximum error of the local regression model is smaller than the response surface model. The points in the residual plot of local regression model is also closer to the zero line, which means that the mean error of local regression model is smaller than that of the response surface model. Therefore, this agrees with the error analysis results.

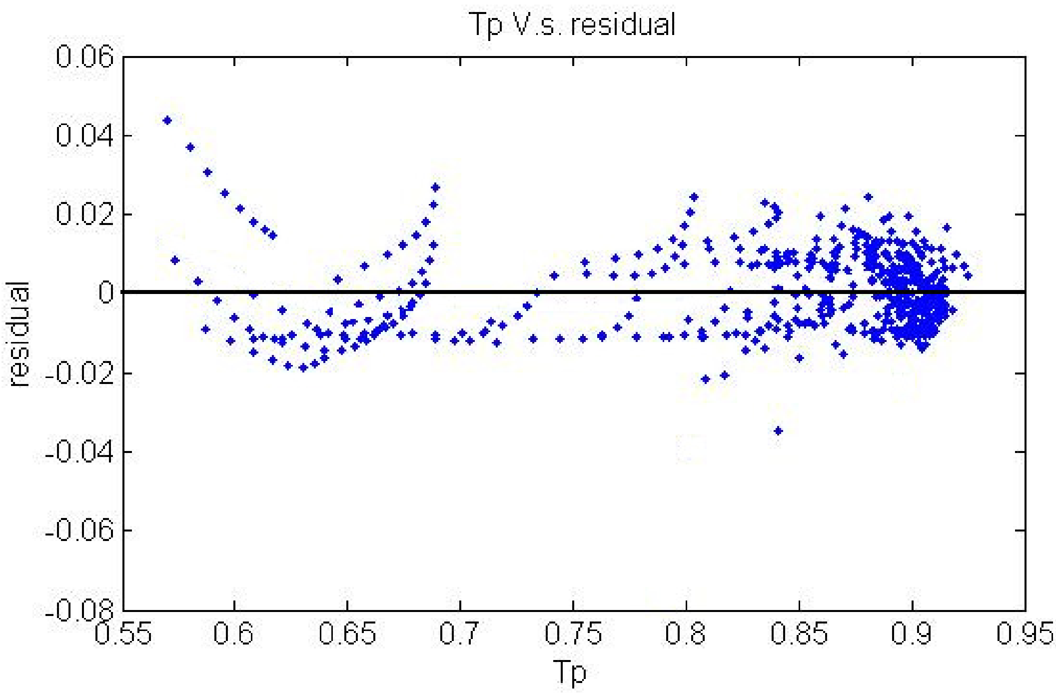


Figure 5. 9 - Residual plot of the local regression model

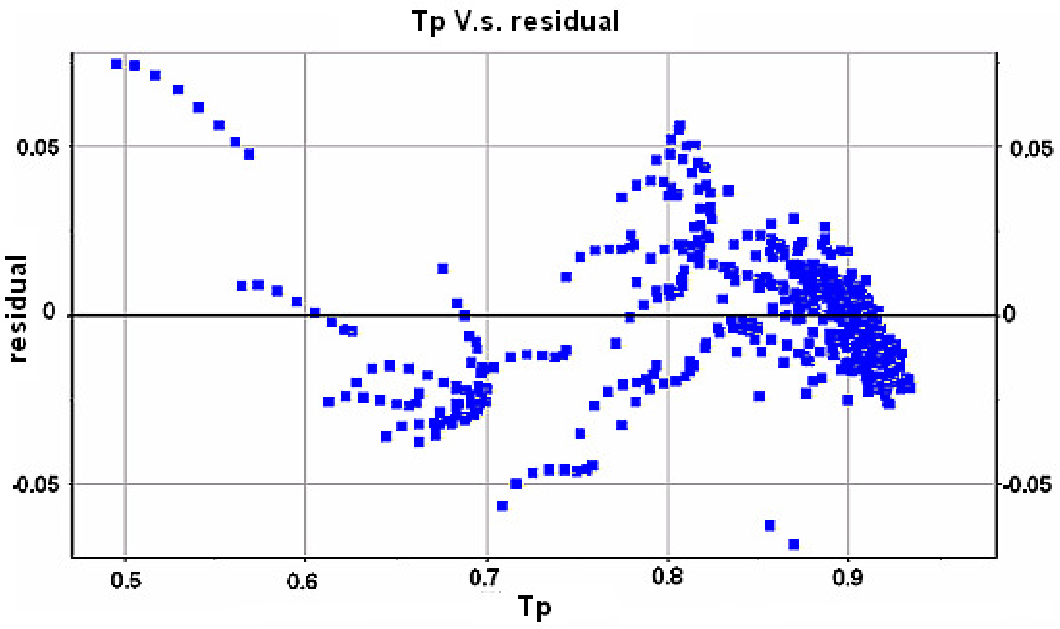


Figure 5. 10 - Residual plot of the response surface model

Graphical Comparison of Response Surface Model and Local Regression Model

The surface plots of the response surface model and local regression model are compared. The surface plot of the local regression model is created based on the meshed prediction points of local regression model rather than based on an explicit function. The surface plots of the local regression model and the response surface model is shown in Figure 5. 11 and Figure 5. 12.

The contours of the response surface model and the local regression model are very similar. However, the local regression model obviously shows more nonlinear details as expected, because the MSE of the local regression model is smaller so that it can represent the observed data better. Therefore, the graphical comparisons also show that the local regression model is more accurate in predicting response than the full cubic response surface model.

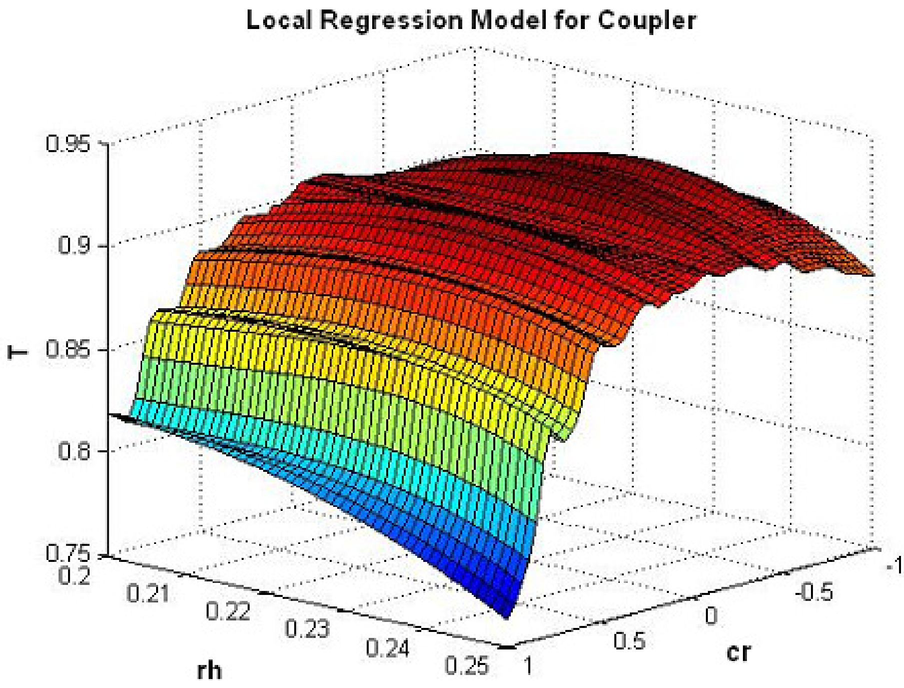


Figure 5. 11 - Fitted Surface of the Coupler Model (when *np*=10)

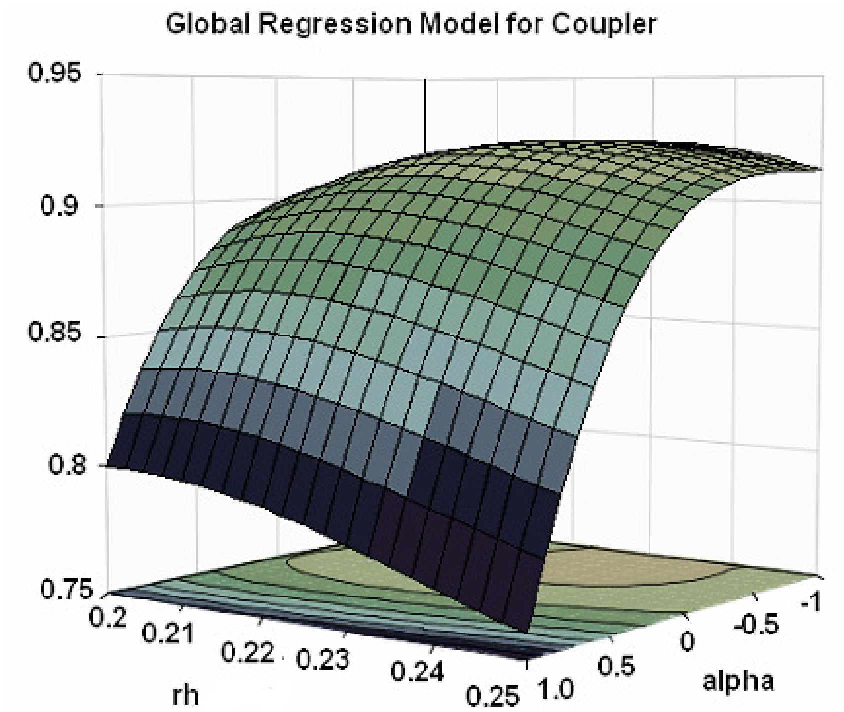


Figure 5. 12 - Response Surface from Global Regression Method (RSM) (when np=10)

5.2.4 Inverse Design Exploration Procedure

After the surrogate models are created, the next step is to implement the inverse design exploration procedure to find a ranged set of solutions robust to the uncertainty in the model chain. In Step 1, the coupler model is the first subsystem to design. According to the design requirement of the system transmission, T_{system}, the ranges of three design variables can be obtained. In Step 2, the waveguide model is the subsystem to design. The intermediate feasible design range of *rh* in waveguide becomes the design bound in this subsystem design range. According to the design requirement of the waveguide transmission, $T_{waveguide}$, the intermediate feasible ranged set of *rh* solutions is further reduced, which is the final feasible design solution for the whole system design problem. In the following sub-sections, the design problems of coupler model and waveguide model are discussed. The steps are presented in Figure 5. 13.

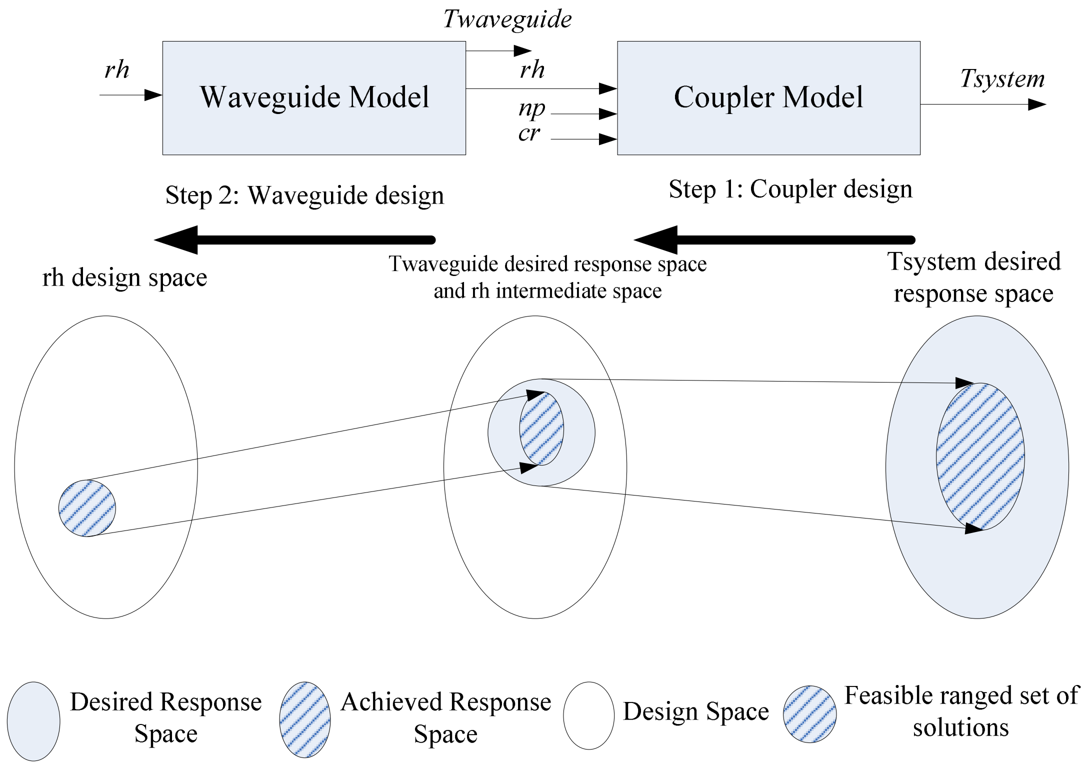


Figure 5. 13 - Inverse design exploration procedure of photonic crystal coupler and waveguide design

5.2.5 Robust Design Solution of PCCW Design Problem

The compromise DSP for the coupler local regression model is shown in Table 5. 2.

Table 5. 2 - Compromise DSP for local regression coupler model

Given

f_c; local regression model for the coupler model;

f_{lc}; 95% lower confidence interval as the lower uncertainty bound function for the coupler model;

$drh = 0.01$; radius of design freedom of *rh*;

$dcr = 0.2$; radius of design freedom of *cr*;

$dnp = 1$; radius of design freedom of *np*;

y_0 Mean response

$Y_{\min} = \underset{[x_i - dx, x_i + dx]}{Min} \{f_c\}$ x_i is the ith design variable;

Feasible transmission must be larger than 91% so that *LRL* is set as 91%;

$\lambda = 1.55 \mu m$ the wavelength the coupler works with;

Target *EMI* is 10 and *EMI* needs to be maximized.

Find

rh initial radius of the holes;

cr the change rate of the size of holes;

np the number of periods;

d_i^+, d_i^- deviation variables.

Satisfy

Goals:

$EMI \ / EMI_{\text{target}} + d_1^- - d_1^+ = 1$

where $EMI \ = \{[y_0 - LRL]/[-Y_{\min} + y_0]\}$

Bounds:

$rh \in [0.20, 0.25]$ μm;

$cr \in [-1,1]$;

$np \in [1,20]$;

Constraints:

$EMI_i > 0$

$d_i^-, d_i^+ \geq 0$

$d_i^- \cdot d_i^+ = 0$

Minimize

$z_1 = d_1^+ + d_1^-$

The computational codes for EMI calculation and deviation function are available in Appendix B.1 and B.2. Pattern search method in Matlab is used to find the mean values of design variable solutions ranges with minimum deviation function. The solution ranges of the coupler model can be obtained based on the mean values and the radius of design freedom. Robust solutions of the local regression coupler model are shown in Table 5. 3 and Table 5. 4. This solution has *EMI* value 2.0882, larger than unit, which means that response range is far from the boundary. The system transmission range is shown in Table 5. 5, which also shows that the response range is far from the desired response boundary and the responses are feasible.

Table 5. 3 - Robust solution of the local regression coupler model

cr (mean)	*np* (mean)	*rh* (mean) (μm)
-0.308	18	0.23

Table 5. 4 - Robust solution range of local regression coupler model

cr	*np*	*rh* (μm)
[-0.508, -0.108]	[17,19]	[0.22,0.24]

Table 5. 5 - The system transmission range of the robust solution of the coupler model

Minimum System Transmission	Mean Transmission	*EMI*
0.9161	0.9217	2.0882

Since the design variable, *rh* is shared by waveguide subsystem, the solution range of this variable becomes the design bound for the waveguide design problem. The intermediate design space is illustrated in Figure 5. 14.

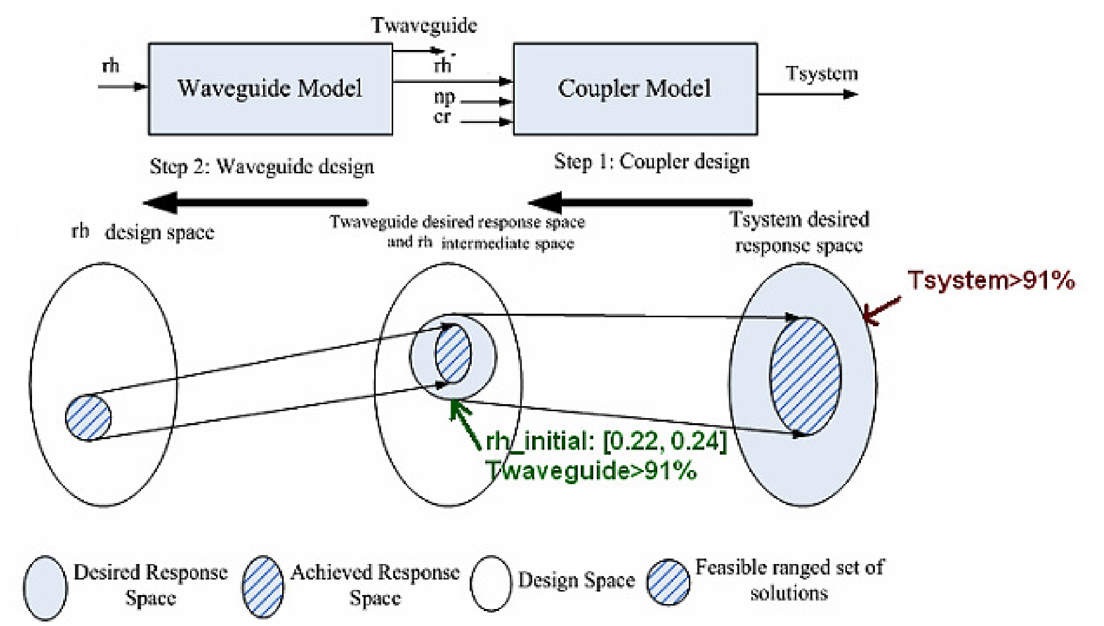


Figure 5. 14 - Intermediate design space of the PCCW design problem

The compromise DSP for the waveguide local regression model is shown in Table 5. 6. Since the initial radius is shared by two models, the initial radius solution with +/- 0.005 deviation range is its design freedom for the waveguide design problem.

Table 5. 6 - Compromise DSP for robust waveguide design

Given f_w; local regression model for the waveguide model; f_{lw}; 95% confidence interval as the lower uncertainty bound of local regression model for the waveguide model; $drh = 0.005$; radius of design freedom of rh; $Y_{\min} = \underset{[x_i - dx, x_i + dx]}{Min} \{f_w\}$ x_i is the ith design variable; Feasible transmission performance is larger than 91% so that LRL equals 91%; $\lambda = 1.55\mu m$ the wavelength the waveguide works with; Target EMI is 5 and EMI needs to be maximized

Find

rh initial radius of air hole in coupler;

d_i^+, d_i^- Deviation Variables.

Satisfy

Goals:

$$EMI \ / EMI_{\text{target}} + d_1^- - d_1^+ = 1$$

where $EMI \ = \{[y_0 - LRL]/[-Y_{\min} + y_0],\}$

Bounds:

$rh\_initial \in [0.22, 0.24]$ μm;

Constraints:

$$EMI_i > 0$$

$$d_i^-, d_i^+ \geq 0$$

$$d_i^- \cdot d_i^+ = 0$$

$$x3 = [0.02, 0.1]$$

Minimize

$$z_1 = d_1^+ + d_1^-$$

The computational codes for EMI calculation and deviation function are available in Appendix B.3 and B.4. Pattern search method in Matlab is used to find the mean values of design variable solutions ranges with minimum deviation function. The ranged set of solutions can be obtained based on the mean values and the radius of design freedom. The ranged set of solutions of waveguide model and response range is shown in Table 5. 7. This solution set has an *EMI* larger than the unit, so that the associated response range satisfies the design requirements and robust to the uncertainty in the model chain. The minimum of the response range is larger than the desired response boundary, which also shows that this ranged set of solutions is feasible. After this step, the design freedom of *rh* is further reduced, which is illustrated in Figure 5. 15, and the ranged sets of solutions for the systems design problem are shown in Table 5. 8.

Table 5. 7 - Robust solution of waveguide model

rh (μm)	*Twaveguide* (mean)	*Twaveguide* (Min)	*EMI*
[0.226,0.236]	0.9285	0.9189	1.9173

Table 5. 8 - Ranged sets of solutions of the whole systems design problem

cr	*np*	*rh* (μm)
[-0.508, -0.108]	[17,19]	[0.226,0.236]

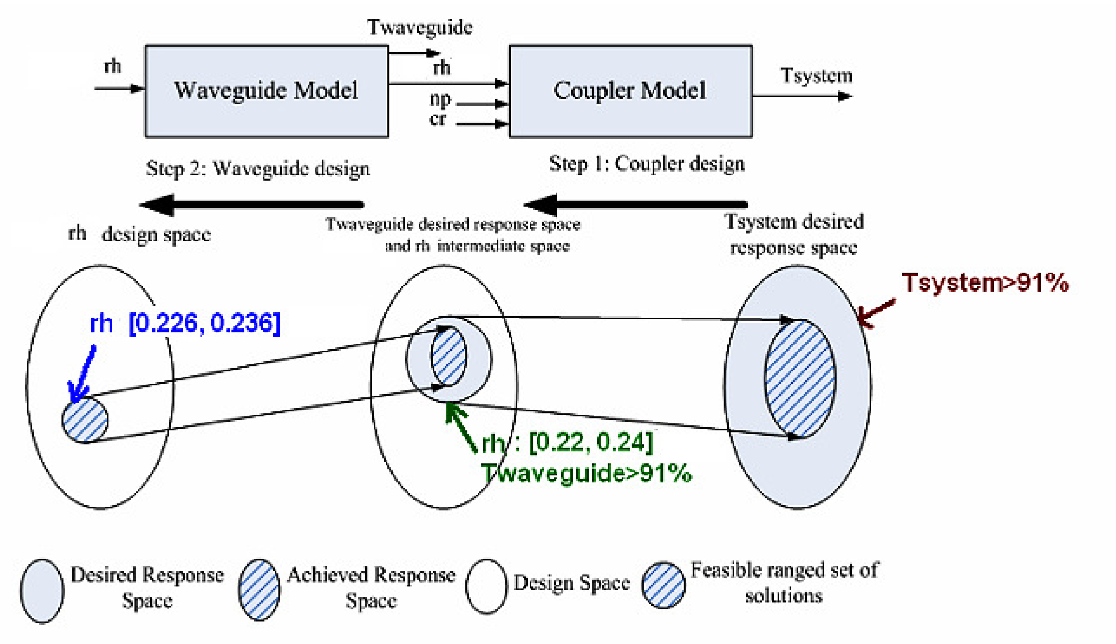


Figure 5. 15 - Change of the design freedom of *rh* through the design process

5.3 NON-ROBUST DESIGN SOLUTION OF PCCW DESIGN

In order to compare the robust solution with non-robust solution, the non-robust design problem of the coupler and waveguide design problem is discussed. In this design problem, the whole system is considered as one system. Therefore, there are three inputs and two outputs in this design problem. The design problem is to optimize two design outputs at the same time. No uncertainty is considered in this problem.

The compromise DSP for the non-robust design of the coupler and waveguide model are shown in the Table 5. 9. Two design objectives are assumed as equally important so that the same weight is given to both design objectives.

Table 5. 9 - Compromise DSP for non-robust PCCW design

Given

Local regression model of the coupler and waveguide;

$\lambda = 1.55\mu m$ the wavelength the coupler works with;

$T_{\text{target}} = 1$ Design target of the system transmission equals to 1.

$Tw_{\text{target}} = 1$ Design target of the waveguide transmission equals to 1;

Find

rh: initial radius of the holes;

cr: the change rate of the size of holes;

np: the number of periods;

Tsystem: the transmission of the system;

Twaveguide: the transmission of the waveguide;

d_i^+, d_i^- Deviation Variables.

Satisfy

Goals:

$Tsystem / Tsystem_{\text{target}} + d_1^- - d_1^+ = 0;$

$Twaveguide / Twaveguide_{\text{target}} + d_2^- - d_2^+ = 0;$

Bounds:

$rh \in [0.20, 0.25]\ \mu\text{m};$

$cr \in [-1, 1];$

$np \in [1, 20];$

Constraints:

$EMI_i > 0$

$d_i^-, d_i^+ \geq 0$

$d_i^- \cdot d_i^+ = 0$

$x3 = [0.02, 0.1]$

Minimize

$Z = Z_1 + Z_2;$

$Z_1 = 0.5 \cdot (d_1^+ + d_1^-)$ deviation function for non-robust design of system transmission;

$Z_2 = 0.5 \cdot (d_2^+ + d_2^-)$ deviation function for optimization design of waveguide transmission;

The pattern search method is used to find the solutions which minimize the deviation function. The non-robust design solution of the PCCW design problem is shown in Table 5. 10.

Table 5. 10 - Non-robust solution of PCCW design

cr	*np*	*rh (μm)*	*Tsystem*	*Twaveguide*
-0.14	20	0.226	0.9230	0.9285

The system transmission of the non-robust solutions is a little larger than the robust solution. This non-robust solution is just close to the boundary of the robust solution space obtained from the DEM-ADS. *cr* and *rh* non-robust solution are located in the feasible range of the robust solution, and only *np* is outside of the feasible range. This means that the response surface is very flat when *np* is from 18 to 20 and the other variables are within the robust solution ranges, shown in Figure 5. 16. Therefore, for this design problem, the response is not adjusted too much for the robustness.

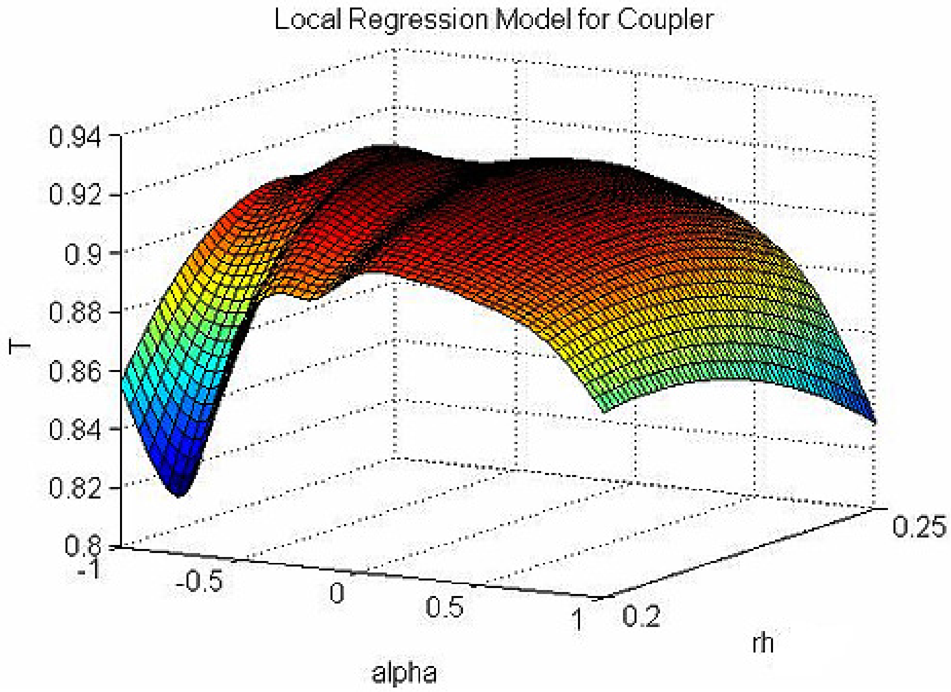


Figure 5. 16 - Response surface of local regression coupler model (*np*=20)

5.4 IDEM DESIGN SOLUTION OF PCCW DESIGN

Since the Hypothesis 1 in this thesis is that the DEM-ADS is more efficient in finding ranged set of solutions than IDEM, it is necessary to compare the solutions and efficiency of both methods. In this section, IDEM was implemented to solve the PCCW design problem.

5.4.1 Design Problem Description for IDEM

Since the waveguide model has only one design variable, the IDEM solution exploration in this problem only focuses on the coupler solution search. According to the IDEM, the first step of the solution exploration is to find out all the feasible solutions. In other word, all of the solutions with EMI value larger than the unit are found out. The compromise DSP for the coupler design problem by IDEM is shown in Table 5. 11.

Table 5. 11 - Compromise DSP for the coupler problem by the IDEM

Given

$HD-EMI_{\text{target}} > 1$; Feasible solutions should have HD-EMIs larger than unit.

$T_w = [0.90, 1]$; the larger waveguide transmission is the better

$T = [0.91, 1]$; the larger system transmission is the better

Variability in *rh*: 0.005 μm; Variability in *cr*: 0.05; Variability in *np*: 2;

Find

rh initial radius of the holes;
cr the change rate of the size of holes;
np the number of periods;
$HD-EMI$

Satisfy

Goals:
$HD-EMI \ / HD-EMI_{\text{target}} + d_1^- - d_1^+ = 1$
Bounds:
$rh \in [0.20, 0.25]$ μm;

$cr \in [-1, 1]$;

$np \in [1, 20]$;
Constraints:
$d_i^- \cdot d_i^+ = 0$;

$d_i^-, d_i^+ \geq 0$;
$Num\{(rh, cr, np)\} \geq 1$

Minimize
$z_1 = d_1^+ + d_1^-$

5.4.2 IDEM Solution of Coupler Design

The basic requirement of the coupler design is that the HD-EMI value should be larger than one. Therefore, the first step of the IDEM solution exploration is to explore the whole design space and find out all the feasible design variables with EMI larger than the unit. The discrete exploration process is implemented to explore the design space, the step size of *rh* is set as 0.005 µm, np is 2 and *cr* is 0.05.

The solution with HD-EMI larger than 1 is illustrated in Figure 5. 17. When the HD-EMI increases to more than 2, the number of the feasible solution points is also reduced, shown as Figure 5. 18. There is no solution when rh equals to 0.21 (mm) and there is one feasible when rh equals to 0.24 (mm). Most feasible solutions are found when rh equals to 0.22 and 0.23 (mm).

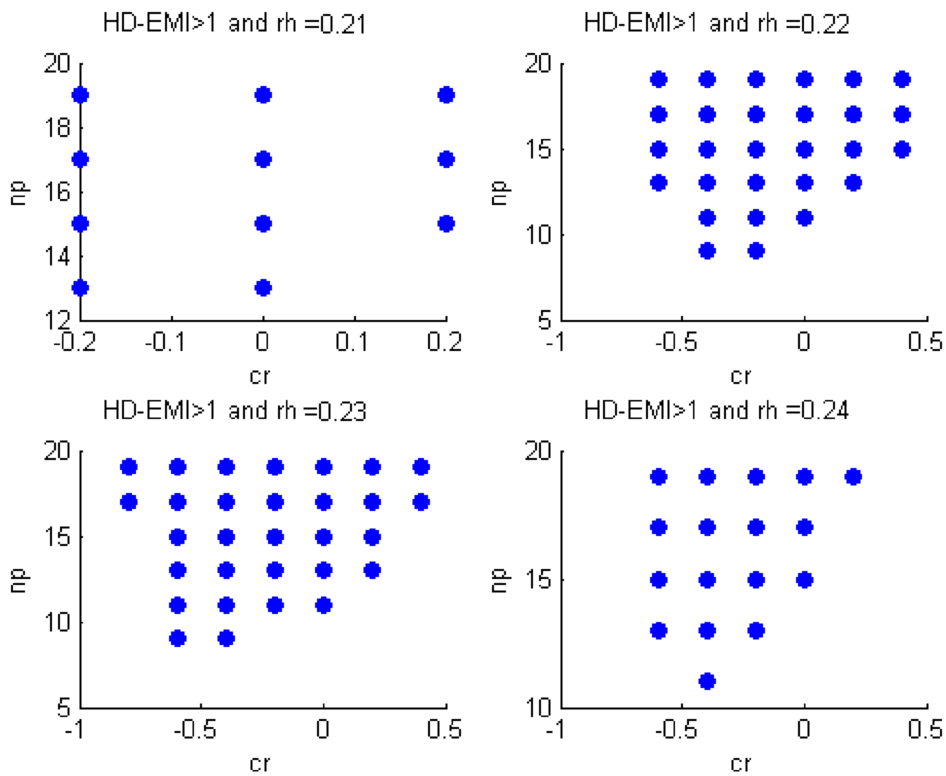


Figure 5. 17 - IDEM solution of the coupler model (*HD-EMI*>1)

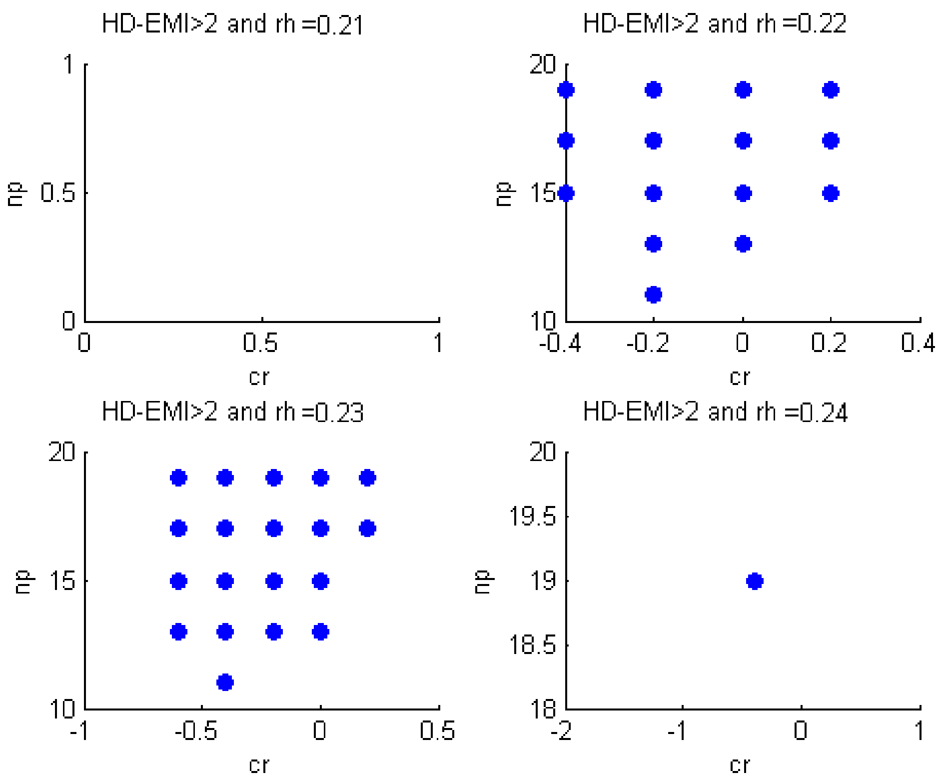


Figure 5. 18 - IDEM solution of the coupler model (*HD-EMI*>2)

Since solutions with *HD-EMI* larger than 2 are good enough, it is not necessary to filter out the solutions with higher *HD-EMI*s. According to the solution plots obtained from the IDEM, *rh* can be 0.22, 0.23 or 0.24; *np* can be from 11 to 19; and *cr* can be from -0.6 to 0.2.

Table 5. 12 - IDEM solution of the coupler model

rh	*np*	*cr*
[0.22, 0.24]	[11, 19]	[-0.6, 0.2]

Compared to the robust solution range obtained from the design exploration method for adaptive design systems (DEM-ADS), the solutions of DEM-ADS is a subset of that of the IDEM. This is expected, because the design exploration principles of two methods are similar, but the IDEM solutions have greater design freedom (larger solution range sizes). However, the computational cost of IDEM solution is also much higher than the DEM-

ADS. As shown in Table 5. 13, the number of calls of the DEM-ADS is much smaller than the IDEM, and the computing time is also less. In terms of this criterion, the DEM-ADS is more efficient in finding solutions than the IDEM.

Table 5. 13 - Comparison of computational cost of two methods in terms of number of calls

Design Methods	IDEM	DEM-ADS
Number of calls	4510	354

5.5 VERIFICATION AND VALIDATION BASED ON THE SIMULATION-BASED PCCW DESIGN

The following section contains evidence for the verification and validation of the design exploration method for adaptive design systems and local regression method presented in Chapter 3 by considering the design of the simulation-based photonic crystal coupler and waveguide. First, the domain-specific structural validity is examined by investigating the appropriateness of the PCCW design problem in adding value to the verification and validation of the DEM-ADS and the local regression method. Then, the domain-specific performance validity of the DEM-ADS and local regression method is examined by looking at the solutions obtained from completing the PCCW example problem in Chapter 5.

Recall the Validation Square discussed in detail in Chapter 2. To summarize, the Validation Square is a construct used in the verification and validation of design methods. In an attempt to facilitate a systematic approach for the validation of design methods, the Validation Square is divided into four sections. Recall that the section of the Validation Square dealing with the application of the proposed design method to example problem including domain-specific structural validity and domain-specific performance validity. In the following sections, ways in which completing the PCCW example problem add value to the domain-specific structural validity and domain-specific performance validity of the developed DEM-ADS are presented.

Both the MESMs example problem (Chapter 4) and the PCCW example problem (Chapter 5) are used in testing the domain-specific structural validity and domain-specific performance validity of the developed DEM-ADS. The MESMs example problem is chosen because it is a well defined multiscale complex system design problem with vertical coupling models introduced in Hae-jin Choi's PhD dissertation [4]. Due to lack of the original model and simulation conditions, the design problem description and meta-models from Dr. Choi's work are used in this thesis, so it is actually a simplified example problem. On the other hand, the MESMs design problem only validates the first hypothesis, the efficiency of the DEM-ADS. The validation of the local regression method is still missing. Therefore, the domain-specific structural validity and domain-specific performance validity are not absolutely satisfied by considering the MESMs design problem. The PCCW example problem is included in this thesis because it is used to illustrate the effectiveness of both the DEM-ADS and local regression method in system design. The result of the MESMs design and the PCCW example problem combine to provide domain-specific structural validity and domain-specific performance validity to the developed DEM-ADS and local regression method.

5.5.1 Domain-Specific Structural Validity

Domain-specific structural validity relates to the appropriateness of the selected example problem and the designer should ask the question "Is the example problem used in demonstrating the method an appropriate choice?" It is asserted that the PCCW example problem is an appropriate choice for testing the effectiveness the DEM-ADS and local regression method because the PCCW problem possesses the following characteristics:

Clearly Defined Adaptive Design Problem

The PCCW design problem contains clearly defined design variables, bounds on design variables, constraints, goals and preferences. Each of these descriptions is necessary for the successful implementation of the DEM-ADS. In addition, both coupler and waveguide simulation models are well defined and tested by Vivek Krishnamurthy during his Ph.D. study [55], so that sufficient design information is available and the design objectives are reasonable. It is not necessary to use discrete exploration process to identify the mapping relationship between the input and output of analysis as the IDEM does. The design problem is also adapted from an existing design problem [55]. Therefore, the PCCW design problem in this thesis is a clearly defined adaptive design problem and it is appropriate to validate the DEM-ADS.

Typical System Design Problem

The PCCW design problem consists of two subsystem models. The two models can be decoupled from the whole system and developed separately. There is a shared design variable in the models. Although this design problem can be solved as a whole system by using other robust design methods, such as RCEM-EMI, it may require higher computational cost and cause difficulty to make collaborative design happen. Therefore, this is a typical system design problem which the design exploration method for adaptive design systems can be used to solve efficiently.

Different types of Uncertainty in PCCW Design Problem

In the PCCW design problem, there are different types of uncertainty. In an attempt to account for design uncertainty without over-complicating the design problem, uncertainty in the design problem is assumed as the random error in the photonic crystal fabrication, the model uncertainty because of the highly nonlinear simulation models. Because models describing the uncertainty in the PCCW design problem are developed, robust design techniques can be employed to develop a robust solution. Robust design is the key element in the DEM-ADS. The PCCW design problem is an appropriate choice in testing this aspect of the developed design approach.

Coupler Model is Nonlinear

The coupler simulation model is nonlinear. A cubic global regression model can only develop a fitting with 95% R-square value, which is not adequate. Therefore, the coupler model is an appropriate example to implement local regression method as model fitting method. The successful implementation of local regression method also adds value to the effectiveness of local regression method in engineering design.

Therefore, the PCCW design problem is an appropriate design example to show the advantage of DEM-ADS in improving the efficiency of solution search and advantage of the local regression method in creating accurate surrogate models than response surface models.

5.5.2 Domain-Specific Performance Validity

Domain-specific structural validity relates to the outcome of applying the method to an example problem and designers should answer the question "Does the application of the method to the example problem produce useful results?". To adequately address this question, two topics are considered: the usefulness of the numerical results and the overall usefulness of the DEM-ADS and local regression method.

Appropriateness of the Accuracy of the Local Regression Coupler Model

The accuracy of the local regression coupler model is test by error analysis. The results show that the accuracy of the local regression is adequate enough to predict the response.

Appropriateness of PCCW Design Solutions

The results are reasonable obtained from the PCCW design problem by the DEM-ADS and local regression method. The solution to design variables and the predicted PCCW performance agree with what is expected. This solution is also approved by the experts in photonic crystal design, Dr. Vivek Krishnamurthy and Dr. Benjamin Klein from Electrical and Computer Engineering Department at Georgia Tech Savannah.

Convergence of the Solution Search

The PCCW example is solved using an optimization routine, pattern search in this thesis. Therefore, it is important to determine whether the optimization algorithm stops at the optimal point or stop because it reaches the maximum number of iterations. The convergence plots of each solution search process are checked as shown in Figure 5. 19 to Figure 5. 21.

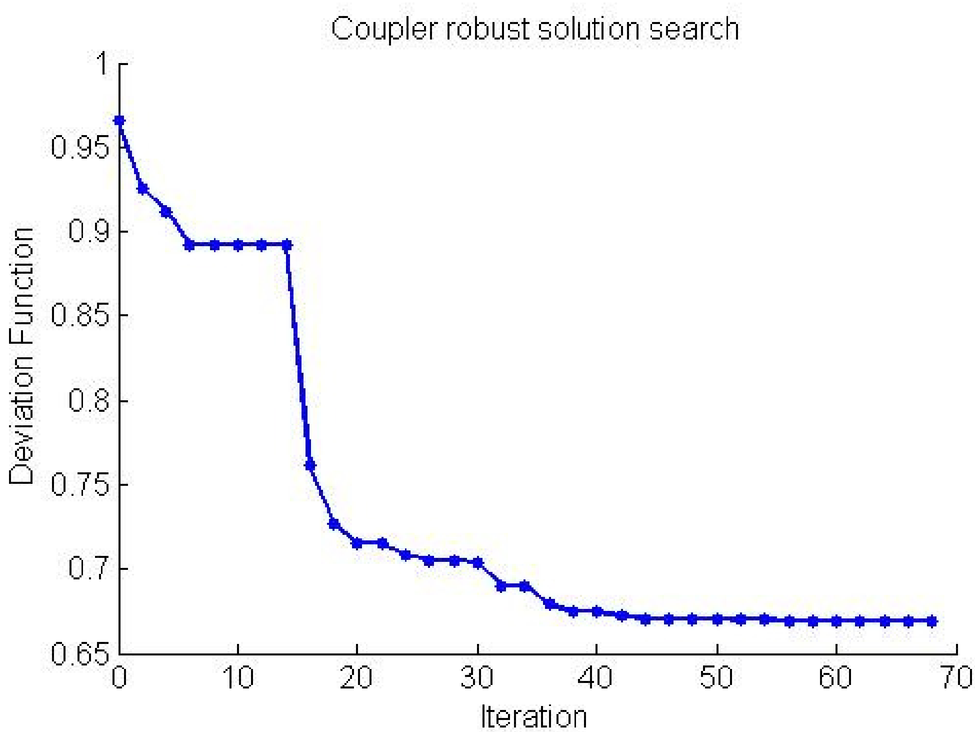


Figure 5. 19 - Convergence plot of coupler robust solution search

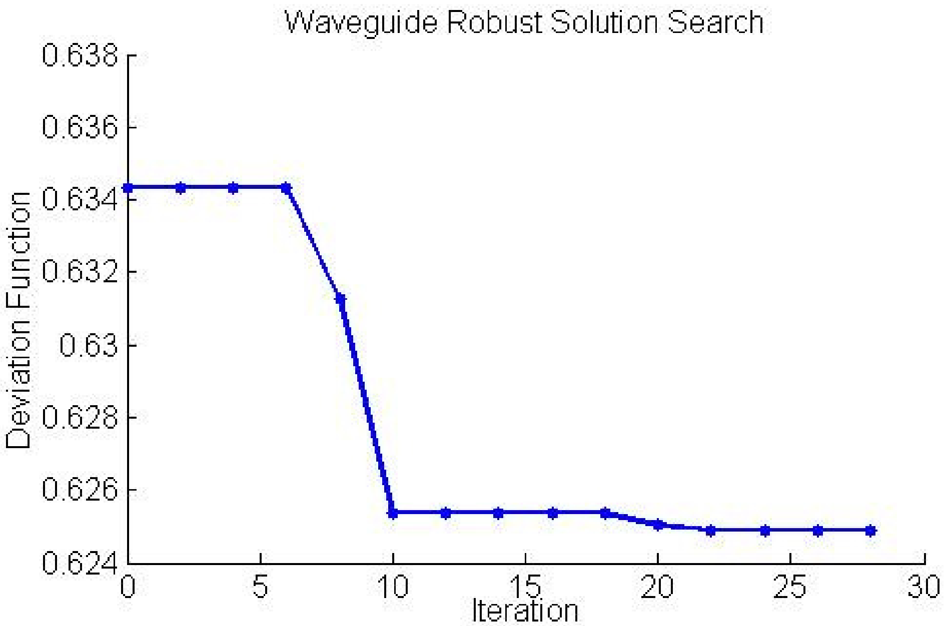


Figure 5. 20 - Convergence plot of waveguide robust solution search

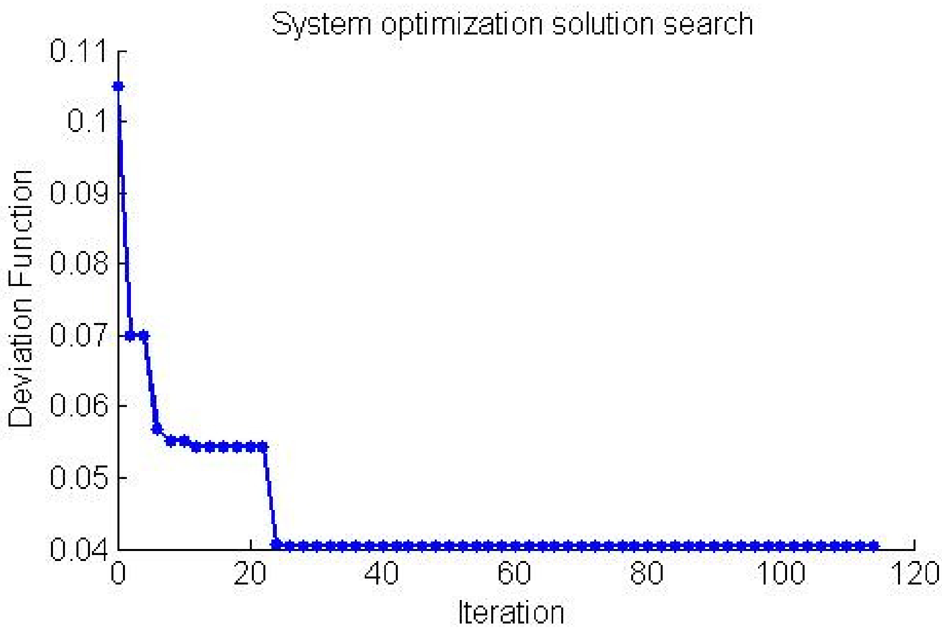


Figure 5. 21 - Convergence of system optimization solution search

The solution search process figures show that all the solution search processes are converged. The optimization processes stopped because the optimum criteria have been reached. Therefore, these results from the optimization routine are acceptable.

Starting Point Analysis for PCCW Design

The internal consistency of the PCCW design solution is also tested with a starting point analysis. The PCCW design problem is solved using an optimization routine. Therefore, it is important to determine if the selected starting point in each solution search results in a robust, stable solution that most closely meets design goals. A starting point analysis that implemented ten different starting points is completed for each solution search. The starting points are at 10% increments of the design variable bounds. The deviation function value is measured at each starting point. The starting point analysis for each solution search is given in Figure 5. 22 to Figure 5. 24.

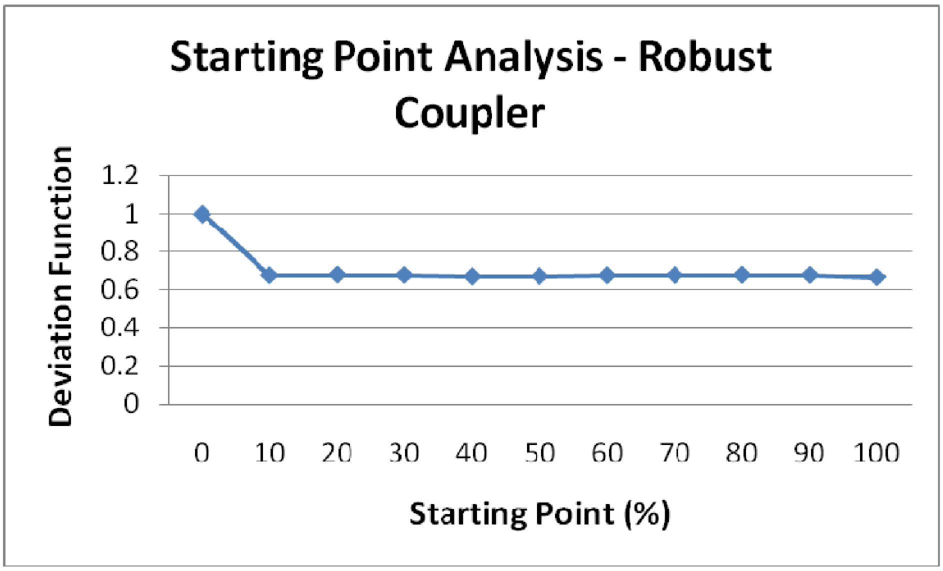


Figure 5. 22 - Starting point analysis of coupler robust solution search

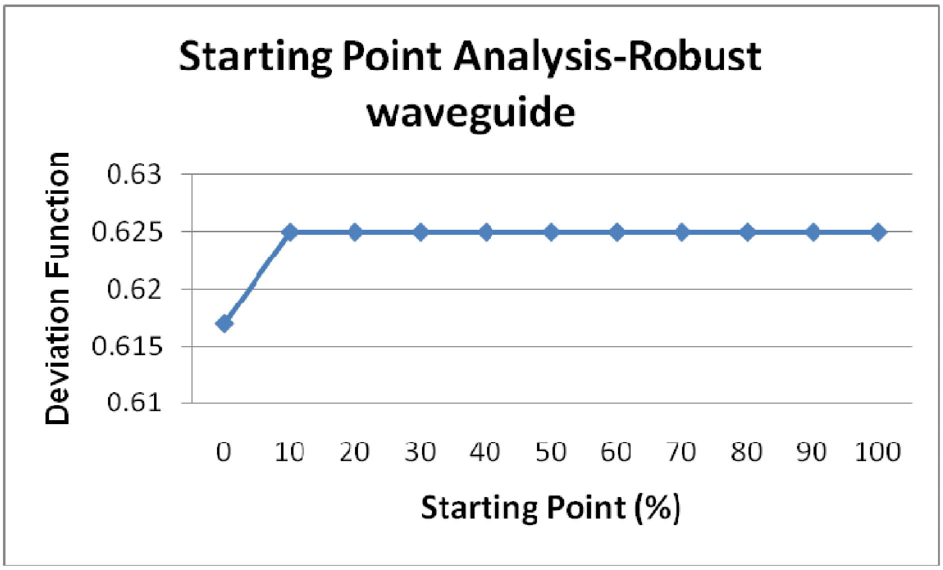


Figure 5. 23 - Starting point analysis of waveguide robust solution search

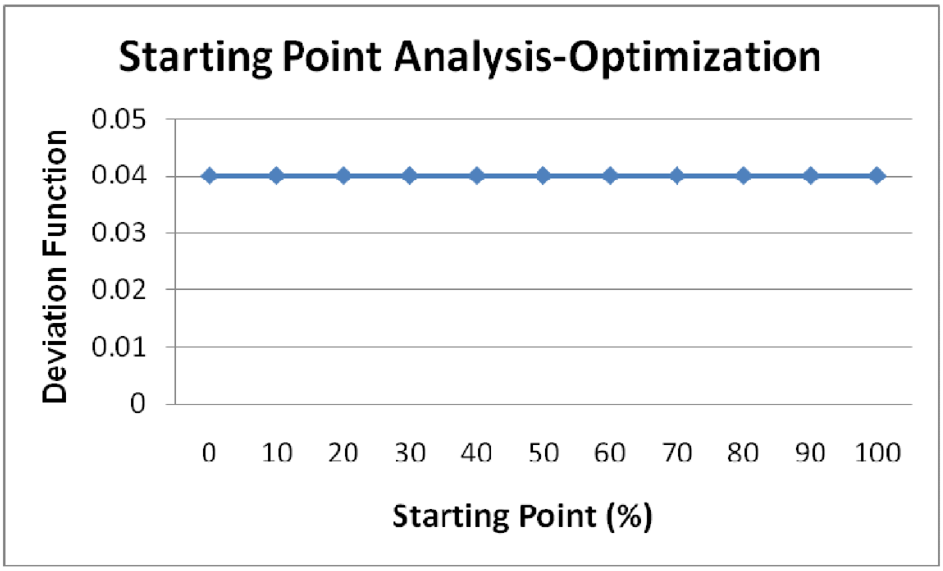


Figure 5. 24 - Starting point analysis of optimization solution search

Both starting analysis results of the coupler model and waveguide model show that the solution is robust to changes in starting points except for the first points (i.e., the boundary). Therefore, the overall robust solution is reasonable. The starting point analysis of the optimal solution search shows that the solution is robust to the changes in all starting points, and the optimal solution is identified.

Usefulness of the Local Regression Method in PCCW Design

Local regression method is very flexible in fitting nonlinear models. The smoothing parameter of the local regression model in the PCCW design is chosen according to the result of the GCV plot. The GCV plot is very useful in helping designers choose the best smoothing parameter. However, designers should have freedom to determine the smoothing parameter according to their own preference, either “honor the data” or “honor the trend”. Therefore, when applying the local regression method in creating surrogate models, designers have much freedom to control the shape of regression surface/ or curve.

In addition, in the PCCW design, both the local regression model and response surface model are used to fit the same DOE data. The error analysis tests show that the local regression model is more accurate than the response surface model in predicting the response. In addition, the graphic comparisons also approve this conclusion. The surface plot meshed by predictions of the local regression model shows more nonlinear features than the response surface model. Therefore, in terms of the prediction error, the local regression model can create more accurate prediction model than the response surface, especially when the original model is nonlinear. The model parameter uncertainty can be reduced by implementation of local regression method.

Usefulness of the DEM-ADS in PCCW Design

The usefulness of applying the DEM-ADS to the PCCW example problem is demonstrated in decreased computation cost. The DEM-ADS solution is a subset of the IDEM solution, it can be considered as the same accurate as the IDEM solution. Although the design freedom of the DEM-ADS solutions is smaller than the IDEM, the computational cost is also much smaller than the IDEM. The computational cost is compared in terms of the number of function calls. The comparisons show that the DEM-ADS need fewer calls to complete the calculation and the computing time is also less than the IDEM. Therefore, it is safe to say that the DEM-ADS is more efficient than the IDEM in this design problem. In addition, due to the implementation of the DEM-ADS, the two subsystem design models are decoupled from the whole systems. The design steps can proceed in parallel or in sequence and the collaborative design can happen. The overall efficiency of design process can be improved.

To summarize, the DEM-ADS and local regression method is a valuable design strategy in the PCCW design problem because the computational cost is decreased and uncertainty existing in the model is also reduced. A visual representation of the value added to the verification and validation of the developed DEM-ADS and local regression method provided in Chapter 5 is shown in Figure 5. 25.

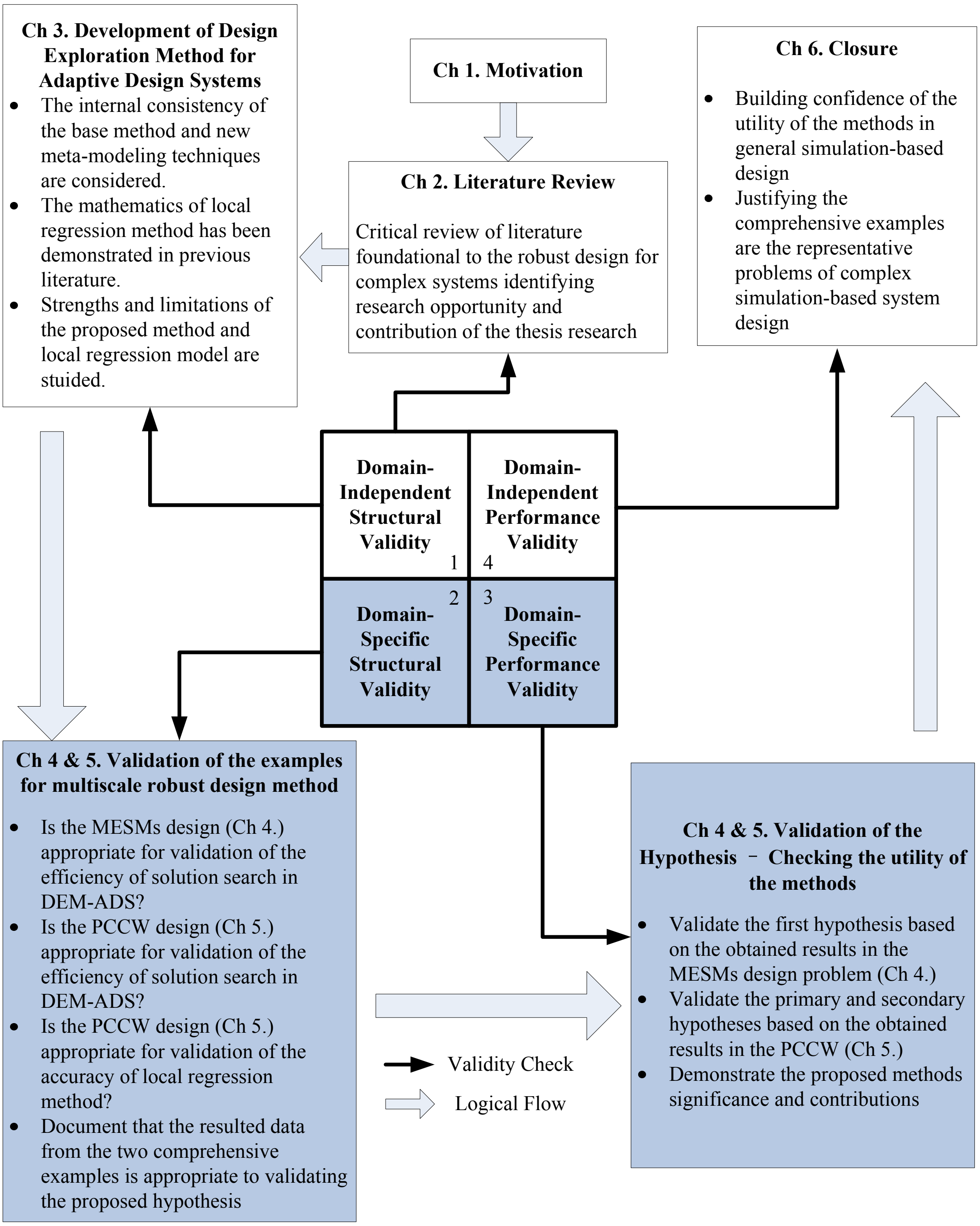


Figure 5. 25 - Value added to verification and validation of the DEM-ADS and local regression method

5.6 SYNOPSIS OF CHAPTER 5

The completion of the PCCW design problem adds value to the validation of the DEM-ADS and local regression method. It is shown that the proposed method can solve systems design problems efficiently, and solutions obtained are robust to uncertainties in the system, which is the primary hypothesis. In addition, it is approved that the accuracy of the surrogate nonlinear model can be improved by using local regression method so that the model uncertainty can be reduced in the system design, which is the secondary hypothesis. In Domain-dependent Structural Validity, it is shown that the PCCW design problem is an appropriate design problem, which is a typical adaptive design system, and this design problem is also appropriate example in which local regression method can create more accurate surrogate model. In Domain-dependent Performance Validity, it is shown that the DEM-ADS solutions are as accurate as the IDEM solution while the efficiency of DEM-ADS design process is much better than IDEM. In addition, it is shown that local regression model has smaller errors than the response surface model according to the error analysis. Therefore, in the PCCW design example, Domain-dependent Structural Validity and Domain-dependent Performance Validity of both primary hypothesis and secondary hypothesis are completed.

In Chapter 6, the thesis concludes with a summary of the validation of the local regression method and DEM-ADS based on the Validation Square. Closing comments relating to the general benefits of the DEM-ADS and local regression method to complex system design, as well as the intellectual contributions presented in this thesis are discussed.

CHAPTER 6
METHOD VALIDATION AND CLOSING STATEMENT

In this thesis, an efficient design exploration method for adaptive design systems is developed for finding a ranged set of solutions against uncertainty in the model chain efficiently. This approach involves an inverse design exploration process modified from the Inductive Design Exploration Method, to improve the efficiency of solution search. For nonlinear subsystem models, the local regression method is introduced as the statistical method for creating accurate surrogate models. The primary contributions are the design exploration method for adaptive design systems and the local regression method which are introduced and developed in this thesis. The design exploration method for adaptive design systems is implemented to facilitate two design problems, MESMs design in Chapter 4 and the Photonic Crystal Coupler and Waveguide design problem in Chapter 5. The local regression method is implemented in the PCCW design and shows the advantages in fitting nonlinear model.

The purpose of this chapter is to bring the development and implementation of this thesis to a close. Closure involves demonstrating that the research questions posed in Chapter 1 are answered in a satisfactory manner. It can be accomplished first by reviewing the validity of the research hypotheses in the context of the validation square, presented in Section 6.1. Then, the achievements and contributions detailed in this thesis are discussed in Section 6.2. This is followed by a critical review of the research presented in this thesis in Section 6.3. Finally, opportunities for future work are discussed in Section 6.4. Chapter 6 in relation to the remainder of this thesis is illustrated in Figure 6. 1.

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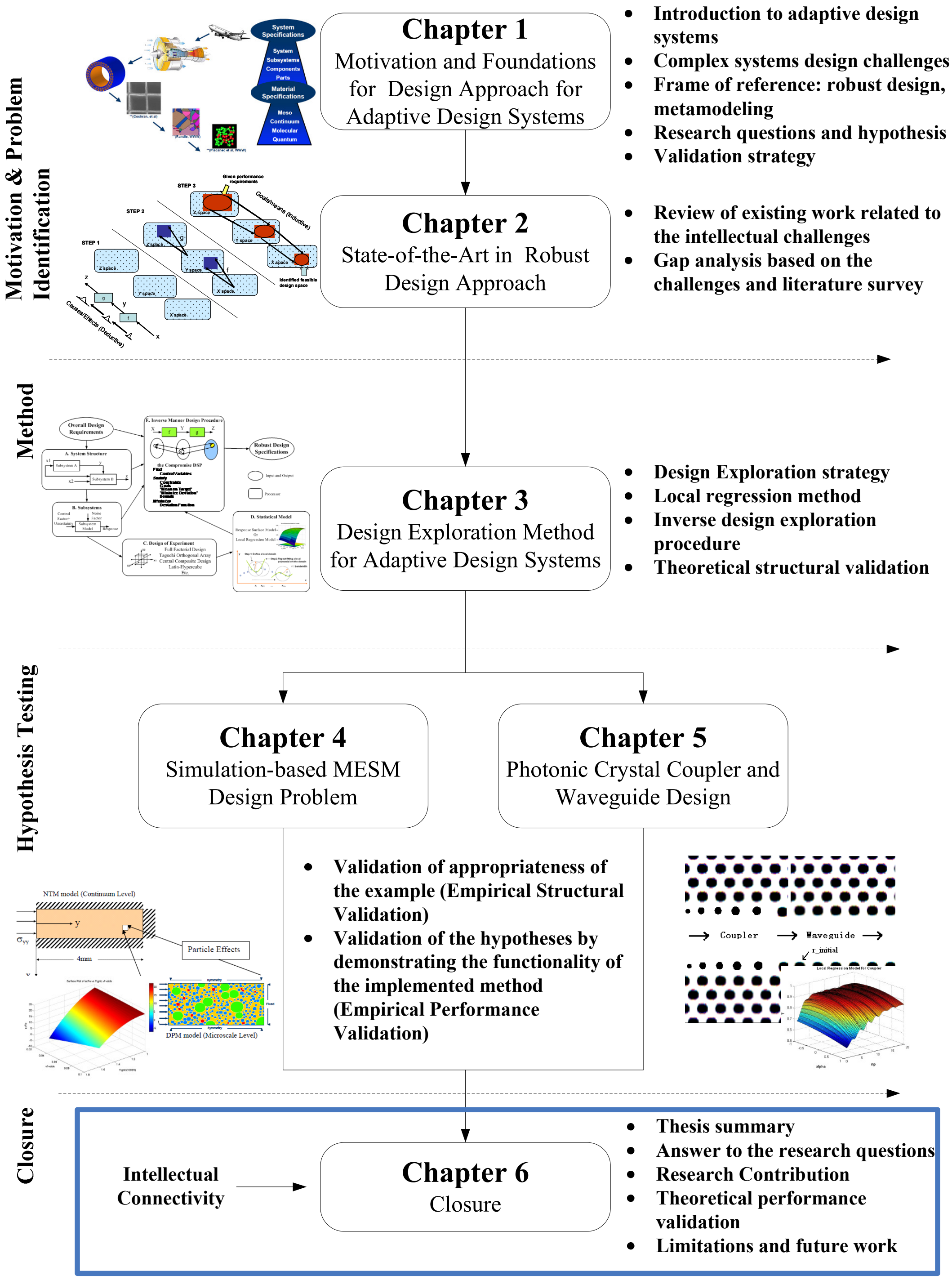

Figure 6. 1 - Thesis roadmap

6.1 VERIFICATION AND VALIDATION OF THE ROBUST DESIGN APPROACH FOR COMPLEX SYSTEMS

In this section, the validation square is used to demonstrate that the methods proposed in response to the research questions in Chapter 1 are valid. In Section 6.1.1, the research questions and hypotheses are revisited. In Section 6.1.2, the hypotheses and associated methods and constructs are reviewed and validated in the context of each quadrant of the validation square.

6.1.1 Revisiting the Research Questions and Hypotheses

Validation in the context of the thesis lies in posing meaningful research questions, proposing answers to the research questions in the form of hypotheses, and demonstrating that the proposed answers are valid. The validation task involves building confidence in the usefulness of the proposed methods for meeting the challenges posed by the research questions. In Section 6.1.2, validation of the research hypotheses is reviewed in the context of the validation square. Before that, the research questions and hypotheses are revisited.

As discussed in Section 1.3.1, a primary research question is addressed in this thesis.

The primary research question to be investigated in this thesis is:

Primary Research Question

How can we control efficiently the uncertainty in the system?

Primary Research Hypothesis

The uncertainty in the systems design environment can be controlled efficiently by the design exploration method for adaptive design systems (DEM-ADS).

The secondary research question to be investigated in this thesis is:

<u>Secondary Research Question</u>

How can the model fitting for highly nonlinear data be improved?

<u>Secondary Research Hypothesis</u>

The model fitting for highly nonlinear data can be improved by the introduction of multivariate local regression into the design process to fit model more accurately.

Answering the research questions involves validating the associated hypotheses which represent answers to the research questions. Aspects of validations are documented throughout the thesis, as outline in Figure 6. 2. In the following section, these discussions of validation are brought together in the context of the validation square and augmented with a discussion of domain-independent performance validity, and the validity of the research hypothesis is asserted.

6.1.2 Testing the Validity of the Proposed Methods

The verification and validation of the design exploration method for adaptive design systems and local regression method is examined using the Validation Square construct. The Validation Square is introduced in Chapter 1 as a systematic procedure for building confidence in the validity of design methods. Evidence for method validation is presented at the end of Chapter 3 – Chapter 5 based on theoretical foundations of the design exploration method for adaptive design systems and local regression method, and successfully application of these methods in example problems. In Chapter 6, aspects of method validation presented throughout the thesis are combined to build confidence in the validation of the proposed methods, shown in Figure 6. 2.

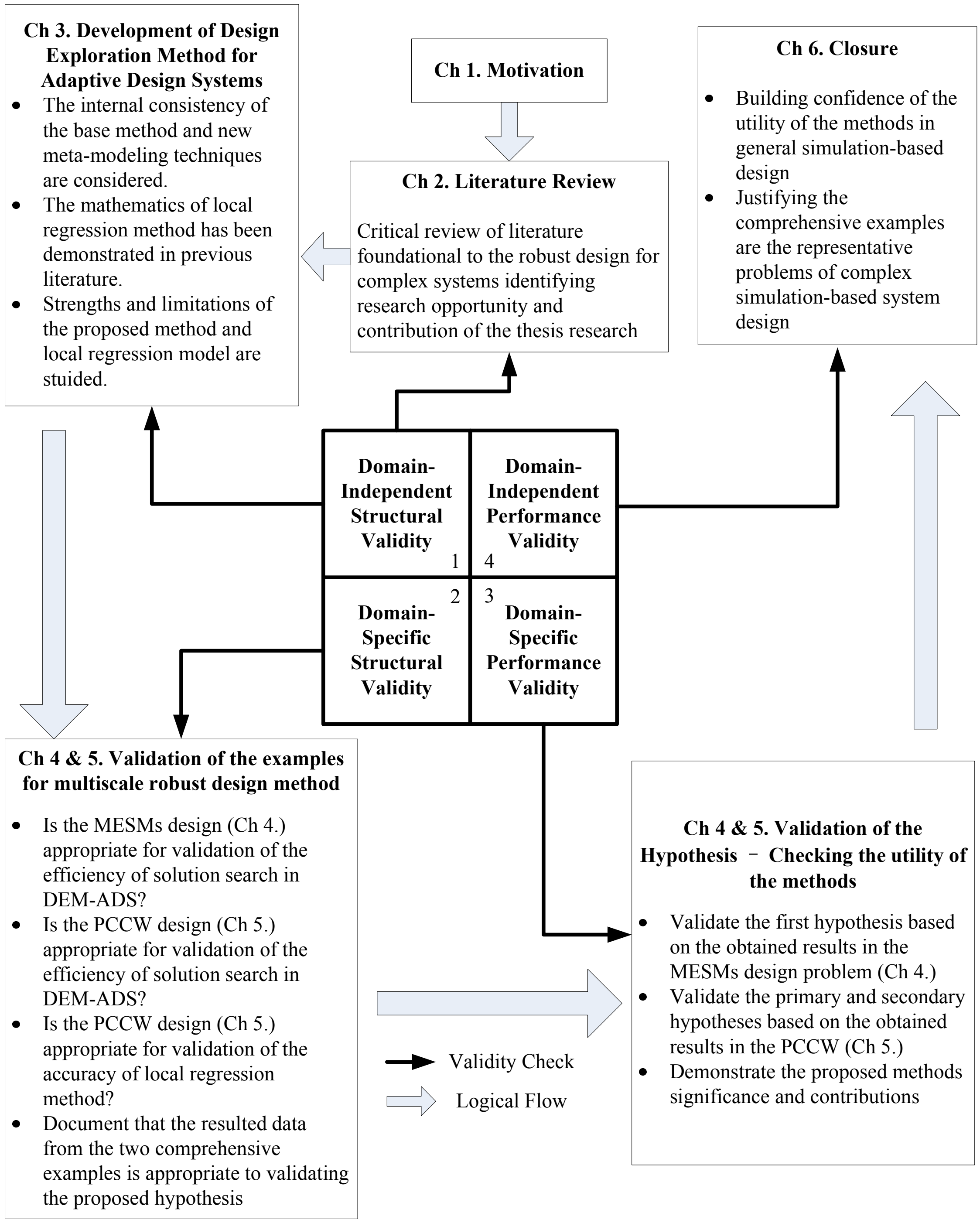

Figure 6. 2 - Thesis validation roadmap

6.1.3 Domain – Independent Structural Validity

Theoretical structural validity involves accepting the individual constructs constituting a method as well as the internal consistency of the assembly of constructs to form an overall method. In this thesis, establishing theoretical structural validity involves searching and referencing the literature related to each of the constructs proposed in the hypotheses. Also, the strengths, limitations, and accepted domain of application of each of the constructs are clearly indicated and supported by argument.

The basic constructs embedded in the research hypotheses are robust design approach for systems design and meta-modeling techniques. The theoretical structural validity of each of the two basic constructs must be tested.

The theoretical structural validity of the basic constructs is established in this thesis as follows:

- The theoretical structural validity of robust design approaches for systems design is established in Section 2.1. This is accomplished by argument and literature review that indicate that Type I, Type II and Type III robust design approaches are effective in finding robust solutions for single design problems, but they do not take the couplings between systems into considerations. The multiscale robust design, the Inductive Design Exploration Method, is effective in exploring feasible solutions robust to uncertainty through the model chain, but the computational cost is expensive. In addition, most robust design approaches implement the response surface model as the meta-modeling technique to reduce the computational cost, but the response surface model is not accurate enough when model is nonlinear. Therefore, it is necessary to explore an alternative meta-modeling technique and identify ways to improve the efficiency of the robust design approaches for systems design.

- The theoretical structural validity of meta-modeling techniques is established in Section 2.2 where it is argued that the meta-modeling techniques are very important in balancing the efficiency and accuracy of solution search in engineering design. Current popular statistical methods, such as the response surface model and kriging, are not satisfactory due to limitations in fitting nonlinear model and sensitivity to the noisy data. Therefore, the accuracy of the meta-model can be improved by introduction of the local regression when simulation model is nonlinear.

- The theoretical structural validity of efficient solution methods is established in Section 2.3 where it is argued that the efficient solution methods, such as Genetic Algorithm, Direct Search, and Adaptive Linear Programming, can be implemented in the robust design approaches for systems design to improve the solution search efficiency. Different solution search methods can be implemented in different cases.

All of these constructs are foundational for the design exploration method for adaptive design systems and local regression method used for nonlinear models, specified in primary and secondary research questions. The domain-independent structural validity of the design exploration method for adaptive design systems is established in Chapter 3. It is argued that the design exploration method for adaptive design systems inherits the basic robust design idea of the IDEM and improves the solution search efficiency. In addition, the appropriate meta-modeling techniques can reduce the model uncertainty in the system. The local regression method is especially useful when the fitting model is highly nonlinear, and this method can effectively reduce the errors in regression models. The solutions obtained with the design exploration method for adaptive design systems are a ranged set of feasible solutions. Designers have freedom to choose the best solutions according to uncertainty condition or other preference.

An information flow chart in Figure 3.11 and the discussion that follows in Section 3.5 builds confidence in the logical progression of thought and information of the design exploration method for adaptive design systems. In Section 3.5, it is verified that for each step in the proposed method there is adequate input information, and that adequate output information is provided for subsequent steps in the design process. Additional confidence is built in the logical information flow of the design exploration method for adaptive design systems in the successful implementation in two example problems (Chapter 4 and Chapter 5). By testing the design exploration method for adaptive design systems using example problems, any inconsistent or illogical information exchange would be indicated by an incomplete or unexpected design solution.

As a result of the theoretical structural validity, confidence has been built in the correctness and consistency of the design exploration method for adaptive design systems and the local regression method in the design process. In addition, the strengths, limitations, and associated domains of application for each method have been identified.

6.1.4 Domain-Specific Structural Validity

Domain-specific structural validity is an analysis of the appropriateness of example problems used to test the effectiveness of the method. Example problems should be similar to the problems for which the method was developed, the example problems should represent actual problems that the method would be applied to, and the example problems should produce useful solutions that can be used to evaluate the effectiveness of the method. Domain-specific validity is established in Section 4.1 and Section 5.1 for the MESMs design and photonic crystal coupler and waveguide design problems, respectively.

First, *are the example problems similar to problems for which the methods proposed in primary hypotheses and secondary hypotheses are generally accepted?* The MESMs design problem is intended to provide support for primary hypothesis. As argued in Section 4.1, the MESMs design problem was a typical multiscale material design problem and now it is a typical adaptive design systems problem after the design problem has been studied by Hae-Jin Choi during his Ph.D. study. The design problem consists of two models at different design scales, so that the uncertainty existing in each subsystem model will be propagated through the design chain. It is necessary to implement robust design approach to find robust solutions against the uncertainty. This design problem is specific for validating the primary hypothesis. As argued in Section 5.1, the photonic crystal coupler and waveguide design problem is also a typical adaptive design systems problem. There are two different simulation models existing in the system with an important coupling, and the subsystem models can be developed separately. The simulation models of the coupler and waveguide have been studied by Vivek Krishnamurthy during his Ph.D. study and the design problem is also adapted from [55] to obtain more accurate solutions. Therefore, the design exploration method for adaptive design systems is appropriate for this example. In addition, the original coupler simulation model is nonlinear and computationally intensive. It is necessary to implement meta-modeling techniques to save the cost. Due to coupler model's nonlinear feature, the response surface model may not provide a satisfactory model with low-order polynomial. Therefore, local regression method is also appropriate to create surrogate coupler model in this design problem. This design problem can validate both hypotheses.

Second, *are the example problems representative of actual problems for which the methods proposed in primary and secondary hypotheses are intended?* As argued in Section 4.1, the MESMs design problem is representative of actual materials design research. This design problem is composed of Reactive Powder Metal Mixtures (RPMMs). It can deliver superior energetic performance, and is unique in that the components serve the dual purpose of providing both energetic fuel and structural integrity to a reactive system [13]. As argued in Section 5.1, the photonic crystal coupler and waveguide design problem is one part of the opto-electronic communication systems design. The robust design is very useful for the photonic crystal because many errors arise from the manufacturing process.

Third, *can the data associated with the example problems be used to support conclusions with respect to primary and secondary hypotheses?* The MESMs design problem is specific to validate the primary hypothesis. The solutions obtained with the design exploration method for adaptive design systems can be compared to the solutions obtained with the IDEM done by Hae-jin Choi. The comparisons can show the accuracy and feasibility of the solution by the proposed method in this thesis. In addition, the number of function calls can be a criterion of computational cost. Such information is available in the computational process of both the IDEM and the design exploration method for adaptive design systems. Therefore, the advantage of the proposed method in efficient solution search can be presented. The photonic crystal coupler and waveguide design problem is proposed to validate both hypotheses. Both the response surface model and the local regression model are implemented to fit the nonlinear coupler model, and the comparisons of error analysis and graphic comparisons can present the accuracy of the local regression model in representing the original models. In addition, the solutions of the design exploration method for adaptive design systems and the IDEM can be compared to show the accuracy and feasibility of the solutions from the proposed method. The computational cost of two methods can be compared in terms of the number of function calls. The comparison results can also show the advantage of the design exploration method for adaptive design systems in solution search efficiency.

Upon answering each of the three questions, the methods proposed in primary and secondary hypotheses are declared domain-specific structurally valid.

6.1.5 Domain-Specific Performance Validity

Domain-specific performance validity is established by applying the method to example problems and testing its effectiveness. Two areas are addressed in order to establish domain-specific performance validity: the usefulness of the numerical design solutions and the overall usefulness of the design exploration method for adaptive design systems and the local regression method. In this thesis, the usefulness of the numerical results is analyzed by conducting starting point analyses and examining the internal consistency of the data.

The MESMs design problem is designed to demonstrate that:

- The design exploration method for adaptive design systems is more efficient in finding solutions robust to uncertainty in the model chain than the IDEM (primary hypothesis).

Domain-specific performance validity with the MESMs design problem is reported in Section 4.4.2. For the MESMs design problem, it is shown that the design exploration method for adaptive design systems can provide similar accurate robust solutions while its computational cost is much less than the IDEM according to the comparisons of the number of function calls.

Usefulness of numerical result in MESMs example problem

The solutions obtained with the design exploration method for adaptive design systems are a subset of solutions obtained with the IDEM. This is reasonable because the design freedom in the design exploration method is reduced in each step, so that the design freedom of final solutions from the design exploration method for adaptive design systems must be smaller than solutions from the IDEM. In addition, since the solutions from the IDEM have been approved by Hae-Jin Choi in his Ph.D. dissertation [4], the solutions in this thesis should also be feasible.

The convergence plot of solution search is implemented to check the feasibility of the solutions. Because the MESMs design problem is solved using an optimization routine, pattern search in this thesis, it is necessary to determine if the optimization algorithm stops at the optimal point or stop because it reaches the maximum of its iterations. The convergence plots in Section 4.4.2 show that all the solution search processes converge. Therefore, these results are feasible.

The internal consistency of the MESMs design solution is also tested with starting point analysis. A starting point analysis that implemented ten different starting points is completed for each solution search. The starting points are at 10% increments of the design variable bounds. The deviation function value is measured at each starting point. The starting point analysis of NTM model design shows that the solutions are robust to changes in starting points so that the solutions are acceptable. The DPM solution search shows high percentage of local minimum results due to special constraint defined in this design problem. Therefore, in this case, the starting points of DPM solution search are set to reflect the expected solution trend according to the IDEM results. The response is robust to the changes near the expected solution. Different starting points which are far from the expected solution are implemented and the results show that all of the deviation function values obtained are larger than that obtained from the points near the expected solution. Therefore, the current solution can be considered as reasonable.

Usefulness of the design exploration method for adaptive design systems in solving the MESMs example problem

The solutions obtained with the design exploration method for adaptive design systems are compared to the solutions obtained with the IDEM. The comparisons show that the solution from the proposed method is a subset of the IDEM solution, so that the accuracy of the DEM-ADS solutions is not compromised. The computational cost is compared in terms of the number of function calls. The results show that the design exploration method for adaptive design systems requests much fewer function calls than the IDEM for solution search. Since the models for calculation are the same in two methods, it is safe to conclude that the design exploration method for adaptive design systems is more efficient than the IDEM in solution search. However, in this design example, it is also shown a limitation in defining the size of design freedom in DEM-ADS. When the design freedom in the MESMs design problem becomes large, no feasible solutions are found. Therefore, designers should accurately define appropriate size of design freedom in each design step. It is quite possible that different sizes of design freedom may be tried before feasible solutions are found, especially when there are a lot of design constraints existing in the design problems. In such cases, it is recommended that the designers use small design freedom first and then enlarge the design freedom to explore the design space again if necessary.

The photonic crystal coupler and waveguide (PCCW) design problem is designed to demonstrate that:

- The design exploration method for adaptive design systems is more efficient in finding solutions robust to uncertainty in the model chain than the IDEM (primary hypothesis).
- The surrogate model for highly nonlinear data can be improved by the introduction of the local regression method into the design process (secondary hypothesis).

Domain-specific performance validity with the PCCW design problem is reported in Section 5.5.2. For the PCCW design problem, it is shown that the local regression method can create more accurate surrogate model in terms of the error analysis, and the design exploration method for adaptive design systems can provide similar accurate robust solutions while its computational cost is much less than the IDEM according to the comparisons of the number of function calls.

Appropriateness of the Accuracy of the Local Regression Coupler Model

The accuracy of the surrogate model created by the local regression method is tested by the error analysis and graphic analysis. The error between the actual response and prediction response is small enough so that the surrogate model can be accepted. In addition, the accuracy of the local regression can also be represented in the feasibility of the final solutions, which is exactly based on the surrogate models.

Appropriateness of PCCW Design Solutions

The solutions of the PCCW design obtained with the design exploration method for adaptive design systems are approved by the experts in photonic crystal design, Dr. Vivek Krishnamurthy and Dr. Benjamin Klein from Electrical and Computer Engineering Department at Georgia Tech Savannah.

The convergence plot of solution search is implemented to check the feasibility of the solutions. Because the PCCW design problem is solved using an optimization routine, it is necessary to determine if the optimization algorithm stops at the optimal point or stop because it reaches the maximum of its iterations. The convergence plots in Section 5.5.2 show that all the solution search processes converge. Therefore, these results are feasible.

The internal consistency of the PCCW design solution is also tested with a starting point analysis. A starting point analysis that implemented ten different starting points is completed for each solution search. The starting points are at 10% increments of the design variable bounds. The deviation function value is measured at each starting point. The starting analysis of the coupler model and waveguide model in Section 5.5.2 show that the solution is robust to changes in starting points except for the first points (i.e., the boundary). Therefore, the overall robust solutions are reasonable.

Usefulness of the Local Regression Method in PCCW Design

In Section 5.5.2, the advantage of the local regression method is discussed. The comparisons of the error analysis show that the local regression model is more accurate in predicting responses than the response surface model. Therefore, there are fewer errors in the local regression model so that the model parameter uncertainty can also be reduced in comparison to the response surface model. The local regression method is especially useful when simulation models are nonlinear model.

Usefulness of the design exploration method for adaptive design systems in PCCW Design

The advantages of the design exploration method for adaptive design systems are discussed in Section 5.5.2. For the adaptive design systems in which sufficient design information is available, the design exploration method for adaptive design systems is more efficient in finding robust solutions than the IDEM. Although the design freedom of the final solutions is smaller, there is no evidence that the small design freedom influences the design performance or designer's decision making.

Since the methods proposed in primary and secondary hypotheses are demonstrated to be useful in terms of designing systems with nonlinear models, it is concluded that the methods are valid in terms of domain-specific performance, for the chosen example problems.

6.1 6 Domain-Independent Performance Validity

Domain-independent performance validity involves establishing that the proposed methods are useful beyond the example problems. It involves showing that the example problems are representative of a general class of problems and that the method is useful for these problem.

As part of domain-independent structural validation, it has been argued that the example problems are representative of a general class of problems. This general class of problems is defined by the following characteristics of the example problems:

For the local regression method:

- The model is nonlinear.
- The data for fitting model is not too much.
- The number of design variables of the model is not too large.

Therefore, the local regression method can be implemented in any design problems specially when the model is highly nonlinear and the number of design variables is not too large. Because the data for fitting models in engineering design comes from the Design of Experiments results, the data set is usually not too large. The second characteristic of the example problem appropriate for local regression is easily satisfied. In the surrogate model creating, the design process is domain-independent. The implementation of the local regression method is not limited in any specific research domain. As long as an accurate surrogate model is necessary in the design, the local regression method can be used. This method can be regarded as a backup method when it is difficult to implement the response surface model to fit a model accurately.

For the design exploration method for adaptive design systems

- System includes several subsystems and couplings.

- Design information is sufficient.
- Simulation model for each subsystem is well studied before.

DEM-ADS is based on two important assumptions. First, the design information should be so sufficient that designers do not need to explore the whole design space by discrete design exploration. Second, the design freedom can be defined by designers in the beginning of each design step. These two assumptions can be achieved in most adaptive design problems. In addition, the design process of DEM-ADS is domain-independent. In this thesis, DEM-ADS is implemented in material design and photonic crystal design. In the design problem, the system is abstracted into a model chain after the system structure is identified. Therefore, this method can be used in any adaptive design problem. Due to the efficient solution algorithm implemented in the solution search, DEM-ADS must be more efficient than the IDEM in any specific adaptive design systems problems, in which designers have sufficient design information.

Upon successful review of the methods proposed in primary hypothesis and secondary hypothesis in the context of the four quadrants of the validation square, it is asserted that the research questions have been answered. *The design exploration method for adaptive design systems developed in this thesis is efficient in finding a ranged set of solutions against uncertainty in the model chain. In this approach, appropriate meta-modeling techniques should be used. For nonlinear simulation models, the local regression method can improve the accuracy of the surrogate models.*

6.2 ACHIEVEMENTS AND CONTRIBUTIONS

As introduced in Chapter 1, the primary research question for this thesis is:

How can we control efficiently the uncertainty in the system?

In response to the primary research question, the design exploration method for adaptive design systems, including the inverse design exploration process modified from the Inductive Design Exploration Method, is developed to control efficiently the uncertainty in the complex system design chains. The unique research contributions inherent in the design exploration method for adaptive design systems are discussed in the following paragraphs.

Improving solution search efficiency in the design process

The computing efficiency is always a serious problem in systems design. The current existing multiscale robust design approach, the Inductive Design Exploration Method, is effective in solving multiscale material design problem, but the computational cost is too expensive. The key research contribution in this thesis is the modifications of the IDEM to improve the solution search efficiency, through replacing the discrete exploration process by the continuous solution search process with defined design freedom. The implementations of the design exploration method for adaptive design systems in two design examples show that the accuracy of solutions is not compromised to the solution search efficiency, as long as the assumptions of the proposed method are satisfied. This contribution provides the opportunities for the proposed method to be implemented in more complex systems problems.

Adapting multiscale materials original design for general adaptive design systems

The Inductive Design Exploration Method (IDEM) is effective for the multiscale robust material original design, so that the discrete exploration process is necessary due to the special challenges in material design. However, most engineering system design problems are not original design. Usually, designers implement existing knowledge or simulation models to complete new design objectives or satisfy new requirements modified from a previous design problems. These engineering design problems can be classified as adaptive design. Due to the sufficient design information, it is easy for designers to predict the performance range of the simulation model so that reasonable design objectives can be defined. In these cases, it is no longer necessary to implement a discrete exploration process anymore, and the modification of this assumption also bring the opportunities to adapt the IDEM for general systems design other than material design domain.

In engineering design prospective, multiscale materials design shares some characteristics of general adaptive design systems, such as multiple interactions between different scales existing in the problem. The multiscale material design focuses more on the multi-level couplings, which happens in different length or time intervals, while both multi-level and single-level couplings are popular in the general adaptive design systems. These problems have the same design challenge, the uncertainty management. The IDEM provides an excellent idea to manage the uncertainty in the model chain, to find a ranged set of solution through a top-down process. This basic idea is also feasible in the general adaptive design problems. Therefore, one contribution of this thesis is to modify the basic idea of robust design to the uncertainty and address the limitations of the discrete exploration process to extend the applications of multiscale material design approach to more general adaptive design systems problems.

As introduced in Chapter 1, the secondary research question for this thesis is:

How can the model fitting for highly nonlinear data be improved?

The second key contribution in this thesis is the introduction and application of the local regression method to the engineering design. Besides the uncertainty from control factors and noise factors, model parameter uncertainty is another important uncertainty caused by inaccurate surrogate models or insufficient knowledge of models. As the same as the uncertainties from control factors and noise factors, it is almost impossible or difficult to eliminate this uncertainty. Therefore, in this thesis, one way to address this limitation is to improve the accuracy of surrogate models in predicting responses. Many robust design approaches implement the response surface model as meta-modeling techniques to replace the original computationally intensive model. However, the response surface model has a serious limitation in fitting nonlinear model. Since many simulation models are highly nonlinear, it is necessary to find an alternative statistical method to address this limitation in engineering design. The answer to the secondary research question in this thesis is the introduction of the local regression method. The local regression method provides designers an alternative to deal with the nonlinear model. Its mathematical foundation is similar to the response surface model, so that it is very easy to use. In addition, it is able to fit nonlinear model with low-order local polynomials better than high order response surface model, in this thesis. With flexible parameter setting, it can also be insensitive to the noisy in the data set. Therefore, the application of the local regression in the engineering design may improve the accuracy of the surrogate model and reduce the model parameter uncertainty in the system.

The third contribution in this thesis is the implementation of the robust design concept in the photonic crystal coupler and waveguide design. In the photonic crystal research field, optimal design methodology is commonly used and assumed that the designed structure is free of any fabrication errors. However, it is demonstrated that extrinsic losses due to fabrication errors are equally important intrinsic losses in the design of nano-scale device [55]. Therefore, the introduction of the robust design concept into the photonic crystal device design makes possible a combination of good opto-electronic device performance and low variations in presence of fabrication uncertainties.

It is important to critically review the preceding accomplishments to recognize the limitations of the constructs proposed and investigated in this thesis as well as the methods and case studies employed in the investigation. In the next section, these limitations are reviewed.

6.3 A CRITICAL ANALYSIS AND REVIEW OF THE LIMITATIONS

In this section, the limitations of the research presented in this thesis are identified. The methods proposed in both primary and secondary hypotheses are evaluated, and their limitations are reviewed. Some of these limitations are associated with potential avenues for future work, as discussed in Section 6.4.

Limitations of the design exploration method for adaptive design systems

The improvement of the solution search efficiency of the design exploration method for adaptive design systems is based on an important assumption: the design information is sufficient. It is assumed that this assumption can be easily satisfied in adaptive design. However, as discussed in Section 1.1.2, there is no explicit boundary between different types of design problems. It is quite possible that a design problem includes both original design and adaptive design. Therefore, it is difficult to evaluate clearly if the design information is sufficient or design objective is definitely achievable. In such cases, designers may have to trade off between the efficiency of solution search and the design freedom of the solution search.

Since it is assumed that design information is sufficient, designers do not need large design freedom to make decisions. In this thesis, the rule for choosing reasonable design freedom is not provided. It is assumed that different problems require different sizes of design freedom in terms of the design requirements, possible parameters modification in detail design and uncertainty prediction. Therefore, it depends on designers' expertise to determine how large design freedom is necessary. For systems problems with intermediate design variables (couplings), small design freedom defined may cause 'no solution' situation in the next step. However, when the design freedom is defined too large, 'no solution' situation may happen in current design step. When design freedom becomes large, more solutions candidates are considered. Thus, it is possible that some infeasible solutions are included in the set of solutions candidates, and then the whole set of solutions become infeasible. "No solution" situation happens. Hence, it is quite possible that designers have to try different size of design freedom when the design problem consists of many couplings. This limitation may be addressed by a guideline which helps designers make decision about how large design freedom is necessary to deal with uncertainty, which is discussed in Section 6.4.

The performance variation is not taken into account in the proposed method. The basic idea of robust design in this thesis is inherited from the IDEM, to find ranged sets of solutions against uncertainty through a top-down design process. This idea of robust design is different from Type I and Type II robust design which is to find design specifications associated with small performance variance. In the IDEM and proposed method, the performance variation is not taken into consideration. Instead, the system performance is kept always feasible in the presence of uncertainty. Therefore, it is quite possible that the design specifications obtained with the proposed method will have large performance variance, although the performance is feasible according to the design requirements.

Limitations of the local regression method

Local regression method is very effective in fitting nonlinear data, but its computational cost is considered as a main limitation. Although current computing technology can address this limitation when the number of design variables and the data set is small, it cannot be guaranteed that this method will still be efficient when there are a large number of design variables.

The other main limitation of the local regression method is that the local regression method does not provide any explicit global functions. Unlike the response surface model, which can be easily represented by a mathematical function, the local regression model may only include a series of local polynomial functions. For some programs, such as the "Locfit" program implemented in this thesis, these parameters are not accessible to a designer. In other words, it is difficult for designers to find these local polynomial functions. Therefore, in order to exchange models, designers have to exchange both the original fitting data set and the computing program. It is not as convenient as the response surface model. In addition, due to this limitation, the local regression model cannot be implemented to some computing programs which require the model mathematical functions as input.

6.4 OPPORTUNITIES FOR FUTURE WORK

There are several potential avenues for extending and supplementing the research in this thesis. Some of them are in response to the limitations cited in Section 6.3.

6.4.1 Future Work Related to Design Exploration Method for Adaptive Design Systems

The first area for future advancement of the design exploration method for adaptive design systems proposed in this thesis is the development of information modeling protocols to identify the system structure and couplings. SysML may be an option. The computer interpretable information model may be connected to the coded design exploration method for adaptive design systems so that designers are able to obtain the complex system structure automatically and execute a top-down robust design process by configuring the network of a design process. The proposed method can be coded as a generalized computer program with SysML, so that it could be easily employed to solve various types of complex system design problems.

The second area is to strategically implement both the IDEM and the design exploration method for adaptive design systems in the systems design. As discussed in Section 6.3.1, it is difficult to clearly define the boundary between the original design and adaptive design. Thus, designers may not easily evaluate whether sufficient design information is available. The best way to address this limitation is to implement both methods for different design steps in the same design problems. Usually, in one complex system design problem, there are different types of design. It is quite possible that some problems are original design while others can be classified as the adaptive design or variant design. Then, designers can implement the IDEM in the original design problems and the design exploration method for adaptive design systems in problems with sufficient information. In addition, the design exploration method for adaptive design systems can be implemented as the preliminary design solution search method to search possible solutions efficiently in some original design problems. The solutions obtained can provide insightful information about possible solutions. As discussed in Section 2.1, the reason to use the discrete exploration is to check whether feasible solutions are available for some uncertain design objectives or strict design constraints. If the design exploration method for adaptive design systems can find some solutions, the designers can focus on the specific part of design space and search larger design freedom. By doing so, the overall computational cost of a system design problem can be reduced. This hypothesis needs to be validated in the future work.

The third area is to take the performance variation into considerations. There are two options: one is to include the performance variation as one design objective, the same as Type I and Type II robust design; the other option is to find the specific robust solutions by Type I and Type II robust design method from the ranged set of solutions obtained from the design exploration method for adaptive design systems. Both options can provide designers with design specifications associated with small response variations. This hypothesis should be validated in the future work.

6.4.2 Future Work Related to the Local Regression Method

Local regression model has not been widely used in the engineering design due to its comparatively high computational cost for design problems with large numbers of design variables. However, due to its good ability in fitting nonlinear model, it is an alternative for designers when fitting models. The efficiency of the local regression method in more complex systems problem still needs to be studied in the future work.

Considering more engineering design problems include customer preference into the design process, and customer survey may also lead to important models in the product development design system. The local regression method can be a powerful tool in providing accurate predictions based on the survey data.

6.4.3 Future Work Related to the PCCW Design Problem

Current Photonic Crystal Coupler and Waveguide (PCCW) simulation models are based on the work of Vivek Krishnamurthy and coauthors [55], and implemented in Matlab. These models represent an approximation of PCCW performance of designed structure. The simulation results need to be verified by the experimental results.

As discussed in Chapter 5, the PCCW design should include fabrication errors, which is common in the photonic crystal fabrication. In this thesis, the uncertainty from the fabrication errors is assumed as the specific variations of design variables. However, for the photonic crystal research field, it is a very interesting research topic that how the change of the specific design variables caused by fabrication errors will influence the final performance. For instance, in this thesis, the only the radius variations of air holes in the coupler and waveguide models are considered. The example does not consider the shape variations due to fabrication errors. In the future work, designers in engineering design can work with experts in photonic crystal research field to solve these problems. The robust design for complex systems will add more value to the photonic crystal research.

Finally, for future work in the PCCW design, it is important to include other design scales in photonic crystal communication systems. Photonic crystal coupler and waveguide design is just a part of whole system design. This design problem can be explored in different scales, such as fabrication scale which includes fabrication models, and system scale which concerns the functions of coupler and waveguide in the whole optic-electronic communication system.

6.4.4 Vision for Systems Design of the Future

Society is currently moving towards a distributed and collaborative social and business environment. With powerful communication technologies, especially internet, the world has become a global village, and Globalization 3.0 [57] has already come. In the future, products are designed not only by a group of designers, but also by individual consumers. Therefore, I think the vision for systems design should consider the both consumer factor and designer factor.

Consumers may join the design process both directly or indirectly. The product development may crowd-source to the whole world, and everyone who is accessible to the design information can work on the problem and propose his/her own solutions. Therefore, in the system design prospective, I think it is necessary to divide the whole product design problem into different modular problems so that some of them can crowd-source to consumers and the rest of them can be solved by company's own R&D team. In the R&D team, the collaborative design process also happens, in which different design groups can work on different design parts. In DEM-ADS, the whole system design problems can be analyzed into different subsystems and couplings, and each subsystem design problem is actually a modular design problem. Therefore, DEM-ADS can be regarded as a basic design process for supporting this kind collaborative design problem. Furthermore, consumers may join the design process indirectly, by consumer surveys or market analysis. The market analysis and surveys are analyzed by designers and consumers' opinion can be found out as important inputs into the design process. In the consideration of current competitive market, consumers' opinions are very important because consumers are more willing to buy products with their preference. Important trends are identified from the survey data, and regression methods are usually used to find such trends. Local regression method introduced in this thesis may be an appropriate regression method to explore such trends accurately, especially when the survey data is highly nonlinear. Therefore, DEM-ADS and local regression method provides a foundation to develop a comprehensive design method to support collaborative design environment with consumers' participation.

About designer factor in future system design, I think it is necessary to explore the coordination of distributed designers and the design information. In many globalized companies, international R&D teams located in different nations are working collaboratively in product development projects. Therefore, it is necessary to coordinate the collaboration and manage the solutions obtained by each design team. The inverse design process in DEM-ADS is a good example of such coordination of collaborative design. The output of top-stream design tasks is also the input of the down-stream design tasks in system design. It seems that each design tasks are based on others' work. However, it does not mean that down-stream design groups have to wait for the results of top-streams. In DEM-ADS, some design groups can work in parallel and the intersection of the solutions obtained from these groups are the results for the model chain. By doing that, the efficiency of the system design exploration can be improved and well organized.

Furthermore, sufficient design information is an important assumption in DEM-ADS proposed in this thesis. It is assumed that in the original design, the design information is not sufficient so that it is necessary to explore the design space to understand specific knowledge. However, original knowledge in one field may not be new in other research fields. In future design environment, it is necessary for innovative design groups to establish a comprehensive database to collect and filter any kind of relative information, especially about the technology development and research institutes or groups, which may be just the “lead user” [58] in the near future. The database is not only a pool of information, but also a sort of design catalog. In other word, efforts should be made on managing the database and sorting the information directly for product development. This database may cost a large amount of maintenance cost, but it is worthwhile to do so. Information would become useful only after being filtered and sorted. Therefore, in the future design, the data management is also essential.

In summary, I think, in the future design, engineering design efforts should come from both designers and consumers. The development of the design method supporting collaborative design in the future should take both designer and consumer factors into consideration.

APPENDIX A

COMPUTATIONAL CODES FOR MESMS DESIGN IN CHAPTER 4

In this appendix, the computational codes for the MESMs design problem in Chapter 4 are provided. All the calculations are completed in Matlab.

A.1 EMI Calculations for NTM Model

This function is used to calculate EMI value for each design variable input. The input of the function is two design variables, X3 and Tignit. The output of the function is the EMI value. The lower requirement limit (LRL) is 5, which is defined in the compromise DSP. The mean response is directly obtained from NTM model function, and the lower bound response, min response, can be obtained through response boundary calculation. The code is shown in the following:

```
function EMI=EMI_NTM(x)
%xx1=X3;
%xx2=Tignit;
xx1=x(1);
xx2=x(2);
mean=NTMmodel(xx2,xx1);% mean response
min=mean-abs(-271+287*xx2-232*2*xx1)*0.02-abs(66.3+287*xx1-46.5*2*xx2)*0.2;
% lower boundary response
EMI=(mean-5)/(mean-min); % LRL=5;
```

A.2 Deviation Function for NTM Model

This function is used to calculate the deviation function for each design variable input based on the EMI calculation. This function calls the EMI_NTM, and the EMI objective is 10, which is defined in the compromise DSP. The code is shown in the following:

```
function z=deviation_NTM(x)
EMI=EMI_NTM(x);
z=1-EMI/10;
```

A.3 EMI Calculations for DPM Model

This function is used to calculate EMI value for DPM model for each design variable input. The input of the function is four design variables, RaAl, RaFe2, Ravoid and Vfvoid. The output of the function is the EMI value. The upper requirement limit (URL) is 1.4, which is defined in the compromise DSP. The mean response, minimum response and maximum response are obtained from the simulation model, w_avg_hot_spot_T function. The EMI calculation is based on these response values. The code is shown in the following:

```
function EMI=EMI_MLDT(x1,x2,x3,x4)
%xx1=RaAl;
%xx2=RaFe2;
%xx4=Ravoid;
%xx3=Vfvoid;
xx1=x1*1e-4;
xx2=x2*1e-4;
xx3=x3*1e-2;
xx4=x4*1e-4;

[avg_T] = w_avg_hot_spot_T([xx1 xx2 xx3 xx4]);
mean=avg_T(1);
min=avg_T(2);
max=avg_T(3);

if mean<1
   EMI=-1;
else
EMI=(1.4-mean)/(max-mean);
end;
```

A.4 Deviation Function for DPM Model

This function is used to calculate the deviation function for each design variable input based on the EMI calculation for DPM model. This function calls the MLDT function, and the EMI objective is 10, which is defined in the compromise DSP. The code is shown in the following:

```
function z=deviation_MLDT(x1,x2,x3,x4)
EMI=EMI_MLDT(x1,x2,x3,x4);
z=1-EMI/10;
```

APPENDIX B

COMPUTATIONAL CODES FOR PCCW DESIGN IN CHAPTER 5

In this appendix, the computational codes for the PCCW design problem in Chapter 5 are provided. All the calculations are completed in Matlab.

B.1 EMI Calculations for Local Coupler Model

This function is used to calculate EMI value for each design variable input. The input of the function is three design variables, alpha, np and rh. The output of the function is the EMI value. The lower requirement limit (LRL) is 0.91, which is defined in the compromise DSP. The mean response is directly obtained from local coupler model function, and the lower bound response, min response, can be obtained through response boundary calculation. The code is shown in the following:

```
function EMI=local_EMI(x)
% x1=alpha;
% x2=np;
% x3=rh;
x1=x(1);
x2=round(x(2));
x3=x(3);
x1lb=x(1)-0.2; % design freedom definition
x1ub=x(1)+0.2;
x2lb=x(2)-1;
x2ub=x(2)+1;
x3lb=x(3)-0.01;
x3ub=x(3)+0.01;

input=patternsearch(@objective_coupler,[x1,x2,x3],[],[],[],[],[x1lb,x2lb,x3lb],[x1ub,x2u
b,x3ub])
Tmin=objective_coupler(input); % obtain response boundary - Minimum response
LRL=0.91; % Lower Requirement Limit
T=local_coupler(x1,x2,x3); % Mean response
Tmean=T(1);
T_lower=Tmean-Tmin;
EMI=(Tmean-LRL)/T_lower;
```

```
function Tlb=objective_coupler(x)
x1=x(1);
x2=x(2);
x3=x(3);
res=local_coupler(x1,x2,x3); % res(1):mean response, res(2):lower boundary response,
res(3): upper boundary response
Tlb=res(2);
```

B.2 Deviation Function for Local Coupler Model

This function is used to calculate the deviation function for each design variable input based on the EMI calculation. This function calls the local_EMI, and the EMI objective is 10, which is defined in the compromise DSP. The code is shown in the following:

```
function z=deviation_coupler(x)
EMI=local_EMI(x);
if EMI<0;
   z=1;
else
z=1-EMI/10;
end;
```

B.3 EMI Calculations for Local Waveguide Model

This function is used to calculate EMI value for each design variable input. The input of the function is the only one design variable, rh. The output of the function is the EMI value. The lower requirement limit (LRL) is 0.91, which is defined in the compromise DSP. The mean response is directly obtained from local coupler model function, and the lower bound response, min response, can be obtained through response boundary calculation. The code is shown in the following:

```
function EMI=local_EMI_waveguide(x)
xl=x-0.005;
xu=x+0.005;
input=patternsearch(@objective_waveguide,[x],[],[],[],[],[xl],[xu]); % obtain response
```

```
boundary
LRL=0.91;
res=local_waveguide(input);
Tlb=res(2) % Minimum response;
T=local_waveguide(x); % Mean response
T_lower=T-Tlb;
EMI=(T-LRL)/T_lower;
```

B.4 Deviation Function for Local Waveguide Model

This function is used to calculate the deviation function for each design variable input based on the EMI calculation. This function calls the local_EMI_waveguide, and the EMI objective is 5, which is defined in the compromise DSP. The code is shown in the following:

```
function z=deviation_waveguide(x)
EMI1=local_EMI_waveguide(x);
if EMI<0;
   z=1;
else
z=1-EMI/5;
end;
```

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